EMSP Research

at

Lawrence Berkeley National Laboratory

and

Lawrence Livermore National Laboratory

June 1999

EMSP Research

Lawrence Berkeley National Laboratory
Lawrence Livermore National Laboratory

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California National Laboratory EMSP Research Projects
Lawrence Berkeley National Laboratory
And
Lawrence Livermore National Laboratory

Introduction

The purpose of this document is to communicate the Environmental Management Science Program (EMSP) research being pursued at the California based national laboratories, Lawrence Berkeley National Laboratory (LBNL) and Lawrence Livermore National Laboratory (LLNL). The information contained in this document is intended for use by technology developers, program managers for the purpose of identifying promising research that have may applications to their particular problems.

This document identifies current Environmental Management Site Technology coordinating Group Technology Needs, fundamental science research needs associated with the STCG needs, and the LBNL and LLNL EMSP research projects which have the potential to address those needs.

Notebook Layout

This document has been organized to provide information on the EMSP research being performed at the California based National Laboratories: Lawrence Berkeley National Laboratory and Lawrence Livermore National Laboratory. It is meant to complement and expand on the other needs notebooks that have been produced to support the integration of EMSP research into the Focus Areas.

Section One contains a listing of the 28 EMSP projects being funded at Lawrence Berkeley National Laboratory and Lawrence Livermore National Laboratory. The associated Environmental Management Problem areas and Science categories are also presented in this listing.

Section Two provides more detailed information on the current EMSP projects at Lawrence Berkeley National Laboratory. The project information and descriptions come from the project abstracts, annual reports, as well as interviews and discussions with the researchers. An attempt has also been made to identify the potential impacts of the research as it applies to the EM program.

Section Three provides more detailed information on the current EMSP projects at Lawrence Livermore National Laboratory. The project information and descriptions come from the project abstracts, annual reports, as well as interviews and discussions with the researchers. An attempt has also been made to identify the potential impacts of the research as it applies to the EM program.

Section Four lists the current LBNL and LLNL projects sorted by OST Focus Area. Within this sorting, the EMSP projects are listed by Science categories. In should be noted that some projects have potential applications in more than one focus area. In these cases, the projects were listed in all the focus areas where they might have potential application.

Section Five is a listing of all the applicable DOE Site Technology Coordination Group Technology needs which the LBNL and LLNL research projects have the potential to address sorted by OST Focus Area. Within each STCG need, the research need associated with that STCG need has been identified and the EMSP project that has potential to address that need has been listed. In this case, the project links take into account the fact that there are multiple aspects to the projects research and that these aspects may cross or include more than one research area.

Section 1:

Listing of EMSP projects at Lawrence Berkeley National Laboratory and Lawrence Livermore National Laboratory

Environmental Management Science Program
Lawrence Berkeley National Laboratory Research Portfolio

Project #	Research Title	Researchers	EM Problem Area	Science Category	Year
54698	Rapid Mass Spectrometric DNA Diagnostics for Assessing Microbial CommunityActivity During Bioremediation	W. Henry Benner - Lead Jennie Hunter-Cevera	Subsurface Contaminants	Analytical Chemistry and Instrumentation - 1^{0*} Microbial Science	1996
55264	Subsurface High Resolution Definition of Subsurface Heterogeneity for Understanding the Biodynamics of Natural Field Systems: Advancing the Ability for Scaling to Field Conditions	Ernest L. Majer - Lead	Subsurface Contaminants	Microbial Science - 1^0 Geophysics	1996
55318	Improved Analytical Characterization of Solid Waste-Forms by Fundamental Development of Laser Ablation Technology	Richard E. Russo- Lead	High Level Waste - 1^0 Decontamination & Decommissioning Mixed Waste	Analytical Chemistry and Instrumentation	1996
55343	Enzyme Engineering for Biodegradation of Chlorinated Organic Pollutants	Peter G. Schultz- Lead	Subsurface Contaminants	Health Science - 1^0 Engineering Science	1996
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Donald J. DePaolo-Lead B. Mack Kennedy Mark Conrad	Subsurface Contaminants	Geochemistry	1996
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Boris Faybishenko-Lead Cristine Doughty Jil Geller Jane C.S. Long	Subsurface Contaminants	Hydrogeology	1996
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Jiamin Wan- Lead Tetsu K. Tokunaga	Subsurface Contaminants - 1^0 Spent Nuclear Fuel	Geochemistry	1996
60141	Gamma Ray Imaging for Environmental Remediation	Paul N. Luke	Spent Nuclear Fuel - 1^0 Decontamination & Decommissioning High Level Waste Subsurface Contaminants	Analytical Chemistry and Instrumentation	1997

* This indicates the primary EM Problem areas and Science Category in which the research was originally placed by the EM Science Staff.
The additional EM Problem Areas and Science Categories represent other areas in which the research has the potential to apply.

Environmental Management Science Program
Lawrence Berkeley National Laboratory Research Portfolio

Project #	Research Title	Researchers	EM Problem Area	Science Category	Year
60296	Research Program to Investigate the Fundamental Chemistry of Technetium	Norman M. Edelstein-Lead David K. Shuh	High Level Waste	Inorganic Chemistry - 1^0 Separations Chemistry	1997
60328	High Frequency Electromagnetic Impedance Measurements for Characterization, Monitoring and Verification Efforts	Ki Ha Lee- Lead Louise Pellerin	Subsurface Contaminants - 1^0 Decontamination & Decommissioning High Level Waste	Geophysics	1997
60362	Ion-Exchange Processes and Mechanisms in Glasses	David K. Shuh	High Level Waste - 1^0 Mixed Waste	Materials Science	1997
60370	Rational Design of Metal Ion Sequestering Agents	Kenneth N. Raymond-Lead	Mixed Waste - 1^0 Decontamination & Decommissioning High Level Waste Nuclear Materials Subsurface Contaminants	Actinide Chemistry 1^0 Separations Chemistry	1997
60387	Distribution & Solubility of Radionuclides & Neutron Absorbers in Waste Forms for Disposition of Plutonium Ash & Scraps, Excess Plutonium, and Miscellaneous Spent Nuclear Fuels	David K. Shuh N. M. Edelstein	Nuclear Materials - 1^0 Spent Nuclear Fuel	Materials Science	1997
60451	Mechanics of Bubbles in Sludges and Slurries	Morton M. Denn Susan J. Muller	High Level Waste	Engineering Science	1997
65015	Three-Dimensional Position-Sensitive Germanium Detectors	Mark Amman- Lead Paul N. Luke	Decontamination & Decommissioning	Engineering Science	1998
65352	Developing a Fundamental Basis for the Characterization, Separation, and Disposal of Plutonium and other Actinides in High Level Radioactive Waste: The Effect of Temperature and Electrolyte Concentrations on Actinide Speciation	Linfeng Rao	High Level Waste	Actinide Chemistry	1998

* This indicates the primary EM Problem areas and Science Category in which the research was originally placed by the EM Science Staff. The additional EM Problem Areas and Science Categories represent other areas in which the research has the potential to apply.

Environmental Management Science Program
Lawrence Berkeley National Laboratory Research Portfolio

Project #	Research Title	Researchers	EM Problem Area	Science Category	Year
65368	Speciation, Dissolution, and Redox Reactions of Chromium Relevant to Pretreatment nd Separation of High-Level Tank Wastes	Linfeng Rao - Lead	High Level Waste	Separations Chemistry	1998
65370	Actinide-Specific Interfacial Chemistry of Monolayer Coated Mesoporous Ceramics	K.N. Raymond	High Level Waste	Actinide Chemistry	1998
65398	Characterization of Actinides in Simulated Alkaline Tank Waste Sludges and Leach Solutions	Linfeng Rao	High Level Waste	Actinide Chemistry	1998

* This indicates the primary EM Problem areas and Science Category in which the research was originally placed by the EM Science Staff. The additional EM Problem Areas and Science Categories represent other areas in which the research has the potential to apply.

Environmental Management Science Program
Lawrence Livermore National Laboratory Research Portfolio

Project #	Research Title	Researcher	EM Problem Area	Science Category	Year
54576	On the Inclusion of the Interfacial Area Between Phases in the Physical and Mathematical Description of Subsurface Multiphase Flow	Andrew 'Andy' Tompson	Subsurface Contaminants	Hydrogeology	1996
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Charles R. Carrigan – Lead G. Bryant Hudson	Subsurface Contaminants	Hydrogeology	1996
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	James G. Berryman - Lead	Subsurface Contaminants	Geophysics	1996
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry Measurements	Gregory Nimz – Lead Marc Caffee Robert Finkel Jeffrey McAninch	Subsurface Contaminants 1^{0*} High Level Waste	Geochemistry	1996
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature Time and Solution Chemistry	Susan Carroll – Lead Carol Bruton	Subsurface Contaminants	Geochemistry	1996
55411	Joint Inversion of Geophysical Data for Site Characterization and Restoration Monitoring	Patricia A. Berge – Lead James G. Berryman Jeffery J. Roberts Dorthe Wildenschild	Subsurface Contaminants 1^{0} High Level Waste	Geophysics	1996
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Cynthia E. Palmer	Decontamination & Decommissioning 1^{0} Mixed Waste Subsurface Contaminants	Separations Chemistry	1997
60118	Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms	Bartley B. Ebbinghaus	Nuclear Materials 1^{0} High Level Waste	Materials Science	1997
60319	Thermodynamics of the Volatilization of Actinide Metals in the High-Temperature Treatment of Radioactive Wastes	Martyn G. Adamson – Lead Bartley B. Ebbinghaus	Nuclear Materials 1^{0} High Level Waste Mixed Waste Spent Nuclear Fuel	Actinide Chemistry 1^{0} Inorganic Chemistry	1997

* This indicates the primary EM Problem areas and Science Category in which the research was originally placed by the EM Science Staff. The additional EM Problem Areas and Science Categories represent other areas in which the research has the potential to apply.

Section 2:

Current Lawrence Berkeley National Laboratory EMSP projects

EMSP Research
Lawrence Berkeley National Laboratory

Project Number: 54698 **Award Year:** 1996

Project Title: Rapid Mass Spectrometric DNA Diagnostics for Assessing Microbial Community Activity During Bioremediation

Researchers: W. Henry Benner, Lawrence Berkeley National Laboratory -Lead
Jennie Hunter-Cevera, Lawrence Berkeley National Laboratory

EM Problem Areas: Remedial Action

Science Categories/ SubCategories: Analytical Chemistry and Instrumentation / Biomedical Instrumentation (primary)
Microbial Science / Microbial Genetics and Instrumentation

URL: http://www.doe.gov /html/em52/54698.html

Synopsis:

Research on evaluating a bioremediation monitoring strategy that relies on an integrated detection scheme using DNA diagnostic procedures and mass spectrometry.

> Objective is to track bioremediation of contaminated soils by measuring the occurrence of genes in soil samples that are known to code for enzymes capable of degrading specific pollutants.

The use of DNA-based procedures for the detection of biodegrading organisms or genes that code for pollutant-degrading enzymes constitutes a critical technology for following biochemical transformation and substantiating the impact of bioremediation. In previous studies, DNA-based technology has been demonstrated to be a sensitive technique for tracking micro-organism activity at the molecular level. These procedures can be tuned to identify groups of organisms, specific organisms, and to detect signals that measure microbial community activity.

Current baseline DNA-based diagnostic procedures, such as the ligase chain reaction (LCR) and the polymerase chain reaction (PCR), rely on gel electrophoresis as a way to score a diagnostic test. These procedures have an advantage in that they can be tuned to identify groups of organisms, specific organisms, and to detect signals that measure microbial community activity. However, these are tedious and slow techniques. This research is investigating the implementation of time-of-flight (TOF) mass spectrometry as a replacement for gel separations because of its speed advantage and potential for sample automation. It is anticipated that if TOF techniques can be implemented in the procedures, then a very large number of microorganisms and soil samples can be screened for the presence of specific pollutant-degrading genes.

The research consists of a two-fold evaluation investigating:

1) the feasibility of replacing the use of gel separations for identifying polymerase chain reaction (PCR) products with a rapid and automatable form of electrospray mass spectrometry, and
2) the use of matrix-assisted-laser-desorption-ionization mass spectrometry (MALDI-MS) as a tool to score oligonucleotide ligation assays (OLA).

This process has the advantage that it can provide the high throughput capability needed to track the course of bioremediation. The technique is also easily adaptable for use in many different types of studies and has the possibility of being used to look for biological materials other than DNA.

Potential STCG Needs addressed

Subsurface Contaminants Focus Area		
Field Office	**STCG Number**	**STCG Title**
ID	ID-S.2.01	Definition of ´Biologically Active Zones´ in Fractured Rock Environments

EMSP Research
Lawrence Berkeley National Laboratory

Project Number:	55264	**Award Year:**	1996
Project Title:	Subsurface High Resolution Definition of Subsurface Heterogeneity for Understanding the Biodynamics of Natural Field Systems: Advancing the Ability for Scaling to Field Conditions		
Researchers:	Ernest L. Majer, Lawrence Berkeley National Laboratory – Lead PI Thomas M. Stoops, Idaho National Engineering and Environmental Laboratory Fred J. Brockman, Pacific Northwest National Laboratory		
EM Problem Areas:	Subsurface Contaminants		
Science Categories/ SubCategories:	Microbial Science / Microbial Transport (primary) Geophysics / Subsurface Imaging		
URL:	http://www.doe.gov /html/em52/55264.html		

Synopsis:
Research is an integrated physical (geophysical and hydrologic) and microbial study using innovative geophysical imaging and microbial characterization methods to identify key scales of physical heterogeneities that affect the biodynamics of natural subsurface environments.

> The overall goal of this research is to contribute to the understanding of the interrelationships between transport properties and spatially varying physical, chemical, and microbiological heterogeneity.

Baseline subsurface characterization technology consists of well logging (seismic single point data) and ground penetrometer. Improved technology and science enables higher resolution of subsurface conditions than available with conventional methods. This research is investigating the inter-relationships between nutrient and microbial presence in an effort to enable higher resolution of subsurface conditions.

The research is being carried out in both the laboratory and DOE sites under natural conditions. It addresses issues that will aid in the understanding of the scales one must sample in order to design effective remediation strategies. New information will be integrated from a number of separate investigations

- Geophysical imaging -
  Geophysics is ideally suited for extrapolating measurements made in a borehole to the large-scale volume away from the hole. With seismic information on location of fractures, layer continuity, layer thickness and other structural and lithologic features, improved predictive models on flow and transport can be developed and applied.

- Microbial characterization -
  These activities are designed to help identify to what extent geophysical and geochemical properties control the spatial variability of microbiological properties. The objective of this work is to characterize small-scale variations in subsurface microbiological properties for the following purposes: providing quantitative estimates (using variogram models) of the spatial variability of these properties; and understanding the relationships between microbiological, physical, and chemical properties (using cross-correlation models)

- Scale effects -
  An additional objective is to determine how the use of different sample supports affects the measurement of microbiological properties. The definition of an appropriate averaging scale is critical in providing more accurate input into predictive models of contaminant transport and will improve the precision of the simulations.

This work is an extension of basic research on natural heterogeneity first initiated within the DOE/OHER Subsurface Science Program (SSP) and is intended to be one of the building blocks of an integrated and collaborative approach with an INEEL/PNNL effort aimed at understanding the effect of physical heterogeneity on transport properties and biodynamics in natural systems. The work is closely integrated with other EMSP projects at INEEL (Rick Colwell et al.) and PNNL (Fred Brockman and Jim Fredrickson).

This research will, by investigating the interrelationships between transport properties and spatially varying physical, chemical, and microbiological heterogeneity, contribute to an improved ability to more accurately characterize and model subsurface conditions. It addresses methodological issues that will aid in the understanding of the scales one must sample in order to design effective remediation strategies.

Potential STCG Needs addressed

Subsurface Contaminants Focus Area		
Field Office	**STCG Number**	**STCG Title**
NV	NV18-9902-04S	Long-Term Monitoring of Upward and Downward Pathways in the Vadose Zone and Closure Caps
RL	RL-SS29-S	Effect of Subsurface Heterogeneities on Chemical Reaction and Transport

EMSP Research
Lawrence Berkeley National Laboratory

Project Number: 55318 **Award Year:** 1996

Project Title: Improved Analytical Characterization of Solid Waste-Forms by Fundamental Development of Laser Ablation Technology

Researchers: Richard E. Russo, Lawrence Berkeley National Laboratory

EM Problem Areas: High Level Waste (primary)
Decontamination and Decommissioning
Mixed Waste

Science Categories/ SubCategories: Analytical Chemistry and Instrumentation / Laser Ablation Techniques

URL: http://www.doe.gov /html/em52/55318.html

Synopsis:
Research to understand fundamental laser ablation sampling processes and to determine the influence of these processes on the analytical sensitivity and accuracy.

Objective of this research is to gain an understanding of the developmental issues that need to be addressed to advance this technology for quantitative characterization applications.

Chemical characterization is listed as the top priority need in every DOE EM major problem area (high-level waste tanks, contaminant plumes, D&D activities, spent nuclear fuel, mixed wastes, landfills, etc.). Baseline analytical quantitative characterization techniques require significant sample preparation. Current analytic techniques require sample dissolutions, they create eliminate additional solvent waste, contaminate equipment, and expose personnel to samples and solvents. Laser ablation has the potential to minimize or eliminate many of these problems.

Laser ablation is a direct sampling and characterization technology; one ablates the sample and characterizes its chemical composition. The sample can be homogeneous, heterogeneous, radioactive, stable, inorganic, organic, biological, sludge, saltcake, soil, etc. Within the EM program, many of the samples will be hazardous. Laser ablation technology provides these capabilities. There is no sample preparation; therefore, laser ablation can eliminate thousands of dissolutions, eliminate additional solvent waste, minimize contamination of equipment, and minimize personnel exposure to samples and solvents.

This EMSP research endeavors to expand the fundamental basis in laser ablation technology for its application to these DOE characterization needs. Laser ablation must be understood on a fundamental level to ensure confidence in chemical characterization of environmental samples. The goal is to develop a fundamental understanding of laser ablation processes, and to determine the influence of these processes on analytical behavior (sensitivity and accuracy) in order to bring this technology to fruition.

Four issues are being studied to improve analytical sensitivity and accuracy:
- time dependent laser removal of mass from a solid sample
- fractionation
- particle generation and transport

- optimization of the inductively coupled plasma - mass spectrometry (ICP-MS) for laser ablation.

Laser ablation is suitable for characterization of tank waste, vitrified waste, high-level waste, subsurface contamination, environmental samples, plutonium disposition, and other EM applications. Also under investigation is the use of laser ablation for characterization of waste during decontamination.

Potential STCG Needs addressed

Field Office	STCG Number	STCG Title
		None identified at this time

EMSP Research
Lawrence Berkeley National Laboratory

Project Number:	55343	**Award Year:**	1996
Project Title:	Enzyme Engineering for Biodegradation of Chlorinated Organic Pollutants		
Researchers:	Peter G. Schultz, Lawrence Berkeley National Laboratory		
EM Problem Areas:	Subsurface Contaminants		
Science Categories/ SubCategories:	Health Science / Molecular, Structural and Genomic Science (primary) Engineering Science / Bioengineering		
URL:	http://www.doe.gov /html/em52/55343.html		

Synopsis:
Research on the development of tailor-made biological catalysts for modifying or degrading halogenated compounds and other environmental pollutants.

> This research involves the protein engineering of existing enzymes and the "creation" of new enzymes (catalytic antibodies) with enhanced dechlorination capability for a wide variety of chlorinated organic pollutants.

Halogenated organic compounds have had widespread use as fungicides, herbicides, insecticides, algaecides, plasticizers, solvents, hydraulic fluids, refrigerants and intermediates for chemical syntheses. As a result, they constitute one of the largest groups of environmental pollutants. Chlorinated organic compounds comprise the largest fraction of these materials, having been synthesized by large scale processes over the past few decades. Their ubiquitous use and distribution in our ecosystem has raised concern over their possible effects on public health and the environment.

The biodegradation potential of halogenated compounds is difficult and not well understood. Biological cleavage of carbon-halide bonds can be achieved by either enzymatic or biocatalytic dehalogenation or by spontaneous chemical dehalogenation of unstable intermediates. This research involves the protein engineering of existing enzymes and the "creation" of new enzymes (catalytic antibodies) with enhanced dechlorination capability for a wide variety of chlorinated organic pollutants. These enzymes could be used as such or could be inserted into microorganisms designed for high activity in contaminated environments.

Development of antibodies that catalyze the hydrolysis of halogenated aromatics will be carried out through a combination of chemical and genetic approaches.

1. One approach involves the generation of selective catalysts by exploiting the large chemical diversity of the immune system to generate enzymelike catalytic antibodies
2. The second approach involves the development of *in vitro* evolution methods to rapidly evolve protein catalysts with selected functions.

The research is attempting to combine the two approaches to generate catalysts for the bioremediation of halogenated aromatics. Specifically, the researchers are developing general selections and screens for identifying novel catalysts from large libraries of antibody mutants. These methodologies are being initially applied to a well-characterized esterolytic antibody 43C9, but if successful, will provide a general approach for evolving a wide range of bioremediation catalysts for the dehalogenation of halocarbons.

Potential STCG Needs addressed

Subsurface Contaminants Focus Area		
Field Office	**STCG Number**	**STCG Title**
AL	AL-07-06-04-SC	In Situ Remediation Of HE, Solvents, VOCs, SVOCs, Heavy Metals, And Landfill Materials

EMSP Research
Lawrence Berkeley National Laboratory

Project Number:	55351 **Award Year:** 1996
Project Title:	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL
Researchers:	Donald J. DePaolo, Lawrence Berkeley National Laboratory – Lead B. Mack Kennedy, Lawrence Berkeley National Laboratory Mark Conrad, Lawrence Berkeley National Laboratory Thomas R. Wood, Idaho National Environmental and Engineering Laboratory Eric Miller, Idaho National Environmental and Engineering Laboratory
EM Problem Areas:	Subsurface Contaminants
Science Categories/ SubCategories:	Geochemistry / Colloidal Chemistry and Transport
URL:	http://www.doe.gov /html/em52/55351.html

Synopsis:
Research on improving methods for characterizing underground contamination sites and for monitoring how they change with time. Particular emphasis is placed on identifying and quantifying the effects of intrinsic remediation, and verifying the efficacy of engineered remediation activities.

The objective is to demonstrate usefulness of isotopic ratio measurements for subsurface characterization and monitoring.

Isotopic measurements of elements like C, O, H, He, Cl, and Sr, which are present in groundwater and soil gas, provide a quantitative measure of material balance. They can be used to identify the sites of origin of contaminants in groundwater, and to determine if contaminants are being destroyed as a result of natural processes or engineered processes. Isotope ratios can also be used to trace the migration of fluids that are pumped down wells to destroy or confine underground contaminants, such as steam and grout, and they can be used to diagnose what chemical reactions are occurring underground and what materials are reacting.

There are many isotopic ratios that can be measured in groundwater and vadose zone gas that could be valuable for characterizing remediation sites and monitoring remediation activities. The researchers are concentrating on a few that are particularly useful for the problems being addressed at the TAN (Test Area North) and RWMC (Radioactive Waste Management Complex) sites of the Idaho National Engineering Laboratory. Isotopes being studied for this research are carbon-13, carbon-14, helium-3, strontium-87, chlorine-37, and oxygen-18.

For this research, the isotopic ratios of specific elements are used in conjunction with water and gas chemistry to determine:

(1) the extent and nature of chemical reactions in the TAN plume and their role in retardation of radioactive isotopes ^{90}Sr and ^{137}Cs and the attenuation of dissolved chlorinated hydrocarbons;

(2) predict the chemical effects of proposed remediation techniques (bioremediation, oxidation, and grout barrier installation) on transport in the plume;

(3) the extent of natural degradation of chlorinated hydrocarbons in the TAN plume, and the transport of gases through the vadose zone from the plume;
(4) the extent of natural remediation and in situ transformations of volatile organic compounds at the SDA site;
(5) the extent of recirculation of surface air during vapor vacuum extraction activities, and how this changes with season and barometric conditions.

The results to date confirm that isotopic analysis of groundwaters and vadose zone gases are useful for diagnosing chemical processes occurring in the subsurface, and tracing the migration of waters from different sources. At both the RWMC and TAN sites there is evidence of biodegradation of organic material in the subsurface, although the evidence to date suggests that the most problematic contaminants are not being degraded at a significant rate.

Potential STCG Needs addressed

Subsurface Contaminants Focus Area		
Field Office	**STCG Number**	**STCG Title**
ID	ID-6.1.04	In-situ Treatment of VOC Contaminated Groundwater in Deep Fractured Rock
ID	ID-S.1.08	Contaminant Transport in a Fractured Rock Vadose Zone
ID	ID-S.2.01	Definition of ´Biologically Active Zones´ in Fractured Rock Environments
OK	OK99-20	Innovative Technology to Investigate Geology and Groundwater Flow Characteristics in Fractured Rock
OR	ORHY-01a	Dense Non-Aqueous Phase Liquid (DNAPL) Source Characterization, Containment, and Treatment

EMSP Research
Lawrence Berkeley National Laboratory

Project Number:	55359	**Award Year:**	1996
Project Title:	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone		
Researchers:	Boris Faybishenko, Lawrence Berkeley National Laboratory - Lead Christine Doughty, Lawrence Berkeley National Laboratory J.T. Geller, Lawrence Berkeley National Laboratory Thomas R. Wood, Parsons Infrastructure and Technology, Inc. R.K. Podgorney, Parsons Infrastructure and Technology, Inc. T.M.Stoops, Idaho National Engineering and Environmental Laboratory Stephen W.Wheatcraft, University of Nevada Maria I.Dragila, University of Nevada		
EM Problem Areas:	Subsurface Contaminants		
Science Categories/ SubCategories:	Hydrogeology / Instrumentation and Modelling		
URL:	http://www.doe.gov /html/em52/55359.html		

Synopsis:
Research on subsurface fluid flow and contaminant transport processes in heterogeneous soils and fractured rock vadose zones.

The objective of this project is to determine if and when dynamical chaos theory can be used to investigate infiltration of fluid and contaminant transport in heterogeneous soils and fractured rocks.

The research approach assumes that spatial heterogeneity and flow phenomena are affected by non-linear dynamics, in particular, chaotic processes. The research examines examine flow and transport through a fractured vadose zone as a deterministic chaotic dynamical process, and develops a model of it in these terms. It first examines separately the geometric model of fractured rock and the flow dynamics model needed to describe chaotic behavior, then puts the geometry and flow dynamics together to develop a chaotic-dynamical model of flow and transport in a fractured vadose zone. The model is then used to predict the long-term bounds on fluid flow and transport behavior, known as the attractor of the system, and examine the limits of short-term predictability within these bounds.

The objective of this project is being achieved through the following activities

1) Evaluation of chaotic behavior of flow in laboratory and field experiments using methods from non-linear dynamics;
2) Evaluation of the impact these dynamics may have on contaminant transport through heterogeneous fractured rocks and soils, and how it can be used to guide remediation efforts;
3) Development of a conceptual model and mathematical and numerical algorithms for flow and transport, which incorporate both: (a) the spatial variability of heterogeneous porous and fractured media, and (b) the description of the temporal dynamics of flow and transport, which may be chaotic; and

4) Development of appropriate experimental field and laboratory techniques needed to detect diagnostic parameters for chaotic behavior of flow.

The scientific significance of the research rests in: (a) the unique non-linear dynamics analysis of data sets such as fracture and matrix flow rates, pressure, and tracer concentrations, and (b) the development of a new dynamical chaotic model for flow and transport in fractured media.

The results of this project are expected to change the conventional approach of using traditional stochastic and/or deterministic methods to predict flow and transport in environmental systems. Because the non-linearity of environmental systems limits their predictability into the future, the research's aim is to determine how far into the future it is realistic to predict the state of the environmental system, what the bounds on the time of contaminant transport are, and how long clean-up can be expected to take. The significance of the research for the DOE will be in the form of technology developed for vadose zone monitoring and in improved vadose zone site characterization and predictability.

Potential STCG Needs addressed

Subsurface Contaminants Focus Area		
Field Office	**STCG Number**	**STCG Title**
AL	AL-09-01-01-SC-S	Transport of HE and Metals in Fractured Rock and Surface Alluvial Systems
AL	AL-09-01-06-SC-S	Issue of Scale in Flow Prediction and Contaminant Remediation in Porous Media
AL	AL-09-01-08-SC-S	Differences Between Saturated and Unsaturated Systems
AL	AL-09-01-10-SC-S	Physics of Fracture Flow and Transport in the Vadose Zone
AL	AL-09-01-11-SC-S	Water Fluxes and Solute Transport in Arid and Semiarid Environments
AL	AL-09-01-12-SC-S	Groundwater-Surface Water Interactions
ID	ID-S.1.07	Facilitated Transport at DOE Disposal Sites
ID	ID-S.1.08	Contaminant Transport in a Fractured Rock Vadose Zone
OK	OK99-20	Innovative Technology to Investigate Geology and Groundwater Flow Characteristics in Fractured Rock
OR	ORHY-01a	Dense Non-Aqueous Phase Liquid (DNAPL) Source Characterization, Containment, and Treatment
OR	ORHY-12a	Active In Situ Dissolved Phase Treatment Systems
RL	RL-SS31-S	Mathematical Formulations of Chemical Reaction/Material Transport
RL	RL-WT053-S	Containment Mobility Beneath Tank Farms

EMSP Research
Lawrence Berkeley National Laboratory

Project Number: 55396 **Award Year:** 1996

Project Title: Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology

Researchers: Jiamin Wan, Lawrence Berkeley National Laboratory - Lead
Tetsu K. Tokunaga, Lawrence Berkeley National Laboratory

EM Problem Areas: Subsurface Contaminants (primary)
Spent Nuclear Fuel

Science Categories/ SubCategories: Geochemistry / Sorption/Desorption

URL: http://www.doe.gov /html/em52/55396.html

Synopsis:
Research on the sorption of contaminants at gas-water interfaces and the possibility of it being a major mechanism controlling contaminant behavior in subsurface environments.

Research has two objectives:

1. To improve basic understanding of contaminant interactions with gas - water interfaces, with emphasis on behavior of mixed contaminant systems.
2. To develop a sorptive microbubble fractionation remediation technique.

While contaminant sorption at mineral surfaces has received much recognition as a major mechanism controlling contaminant behavior in subsurface environments, virtually no attention has been given to the possibility of contaminant sorption at gas-water interfaces. Moreover, no effort has yet been advanced to optimize such interactions for the purpose of facilitating in-situ remediation. Gas-water interfaces, unlike water-solid interfaces, are mobile. Therefore, associations of contaminants with gas-water interfaces can be very important not only in subsurface contaminant distributions, but also in contaminant transport, and potentially in remediation.

The research is testing three hypotheses in support of the research objectives:

1) Contaminants and natural organics can sorb on and alter the interface hydrophobicity of the gas-water interfaces, and therefore influence sorption of colloids, metals, and radionuclides at gas-water interfaces;
2) Surfactants can vastly increase sorption of colloids, metals and radionuclides selectively onto gas-water interfaces;
3) A sorptive microbubble fractionation remediation technique can be developed based on understanding of contamination interaction with gas-water interfaces.

These hypotheses are being tested through quantification and visualization at both micro- and macro-scales.

In principle, sorptive bubble and microbubble separation techniques can be employed for removing any contaminants that partition favorably at gas - liquid interfaces, in environments that do not severely constrain bubble or microbubble movement. A main focus of this research is identifying surfactants that are highly selective for specific contaminants.

In subsurface environments, the *in-situ* microbubble technique is expected to permit access to contaminated zones that are not pore size-restrictive. Thus, aquifer strata comprised of sands or gravel will be accessible. Additionally, sorptive, mobile gas - liquid interface might be useful in separations in waste tanks. In such an application, either microbubbles or bubbles could be used, since pore-size limitations do not exist. Factors that will determine applicability of this remediation approach include the level of contaminant-surfactant selectivity, microbubble (or bubble) stability and mobility, cost of surfactants, and development of microbubble (or bubble) collection-treatment methods.

Potential STCG Needs Links

Deactivation & Decommissioning Focus Area		
Field Office	**STCG Number**	**STCG Title**
ID	ID-S.2.05	Understanding the Physics and Chemistry of Concrete Decontamination
Mixed Waste Focus Area		
Field Office	**STCG Number**	**STCG Title**
ID	None	Metal ion binding in sludges, sediments and soils
Subsurface Contaminants Focus Area		
Field Office	**STCG Number**	**STCG Title**
AL	AL-07-04-01-SC	Non-Itrusive Removal of Polychlorinated Biphenols (PCBs) from Soil Both Above and Below the Water Table Underneath Buildings
AL	AL-07-06-04-SC	In Situ Remediation Of HE, Solvents, VOCs, SVOCs, Heavy Metals, And Landfill Materials
ID	ID-S.1.08	Contaminant Transport in a Fractured Rock Vadose Zone
ID	ID-S.2.03	Aqueous Transport of Soluble Radionuclides and Heavy Metals: Evaluation of Non-Equilibrium Processes and Native Surfaces in Porous Media

EMSP Research
Lawrence Berkeley National Laboratory

Project Number: 60141 **Award Year:** 1997

Project Title: Gamma Ray Imaging for Environmental Remediation

Researchers: W. Neil Johnson, Naval Research Laboratory - Lead
Paul N. Luke, Lawrence Berkeley National Laboratory
Bernard F. Phlips, Naval Research Laboratory
R. A. Kroeger, Naval Research Laboratory
G. W. Phillips, Naval Research Laboratory

EM Problem Areas: Spent Nuclear Fuel (primary)
Decontamination and Decommissioning
High Level Waste
Subsurface Contaminants

Science Categories/ SubCategories: Analytical Chemistry and Instrumentation / Sensors and Techniques

URL: http://www.doe.gov /html/em52/60141.html

Synopsis:
Research on the development of year development program to apply high resolution gamma-ray imaging technologies to environmental remediation of radioactive hazards

> The objective is to develop high resolution germanium detector systems for direct imaging of spent nuclear fuels and fissile materials and Compton scatter imaging of large objects of arbitrary size.

High resolution, position-sensitive germanium detectors are being developed at the Naval Research Laboratory for space applications with support from the Office of Naval Research and the National Aeronautics and Space Administration. For the EMSP, the researchers will model the performance of these detectors for the following:

- direct imaging of spent nuclear fuels and fissile materials and Compton scatter imaging of large objects of arbitrary size,
- to investigate fabrication of field-usable detectors, and
- to demonstrate the performance of such a system using a small configuration of detectors.

Potential STCG Needs addressed

Deactivation & Decommissioning Focus Area		
Field Office	**STCG Number**	**STCG Title**
ID	ID-7.2.09	Develop a Rapid Wood Radiological Contamination Monitor
RL	RL-DD023-S	Cesuim Source Identification

Subsurface Contaminants Focus Area		
Field Office	**STCG Number**	**STCG Title**
AL	AL-09-01-27-SC-S	Long-term Monitoring Sensor Technology
ID	ID-6.1.01	In-Situ Debris Characterization for Partial Retrieval

EMSP Research
Lawrence Berkeley National Laboratory

Project Number: 60296 **Award Year:** 1997

Project Title: Research Program to Investigate the Fundamental Chemistry of Technetium

Researchers: Norman M. Edelstein, Lawrence Berkeley National Laboratory - Lead
Carol J. Burns, Los Alamos National Laboratory
David K. Shuh, Lawrence Berkeley National Laboratory

EM Problem Areas: High Level Waste
Science Categories/ SubCategories: Inorganic Chemistry / Solid/Solution Chemistry (primary)
Separations Chemistry / Technetium Chemistry and Separations

URL: http://www.doe.gov /html/em52/60296.html

Synopsis:
Research addressing characterization of Technetium (Tc) chemistry pertinent to waste tank environment and various waste forms.

> The objective of this research is to address the fundamental solution chemistry of technetium in the waste tank environment, and in a second part, the stability of Tc in various waste forms.

Technetium (^{99}Tc, ß emitter, half-life 2.1 x 10^5 years, spA= 1.7 x10^{-2} Ci/g) is one of the radionuclides of major concern because of regulatory considerations for radioactive waste disposal. The propensity of Tc as pertechnetate, TcO_4^-, to migrate in the geosphere necessitates its safe, long-term immobilization. Technetium is found in the nuclear waste storage tanks at the Hanford and at the Savannah River sites in highly alkaline environments along with multi-molar concentrations of nitrate, nitrite, and Na ions and lesser amounts of organic complexants, phosphate, sulfate chloride, fluoride, and carbonate. It has been assumed that technetium is present in the waste tanks as the pertechnetate ion but a recent study has suggested that at least in part, technetium is present in another form. There is a lack of information on Tc chemistry in oxidation states III-V with simple inorganic (OH^-, CO_3^{2-}, PO_4^{3-}, SiO_4^{4-}) and common organic ligands (EDTA, citrate, oxalate) under alkaline conditions. This is essential information needed for pretreatment schemes, processing, and the assessment of stability of Tc in waste form materials. Further complicating the Tc waste tank chemistry is the added effect of an intense radiation field originating from ^{137}Cs and ^{90}Sr. The interactions of the ionizing radiation with water, nitrate, nitrite, and other minor components create highly reactive species that can strongly perturb the oxidation-reduction conditions.

The stability of Tc in waste form materials is of paramount importance for long term storage concerns and the solid state chemical properties of many candidate Tc compounds are unknown. There have been few systematic studies of Tc stability in lower valent solids with the exception of TcO_2. Thus, it is not possible at present to assess the long term stability of many Tc compounds relevant to proposed waste form materials.

Research investigating the fundamental solution chemistry of Technetium is pursuing several tracks:

- The solution and solid state chemistry of this element will be studied in aqueous solutions as a function of pH with the various salts added such as nitrate and nitrite, and as a function of radiation dose, to determine if radiolysis effects cause the reduction of the TcO_4^-.

- Search for stable, lower valent forms of Technetium materials that may be thermodynamically and/or kinetically stable and may be incorporated in various waste forms for long term storage. This phase of the program will address the problem of the possible oxidation of low solubility lower valent compounds of Tc in various waste form matrices and the subsequent leaching of highly soluble TcO_4^-.

Based upon the premise that insolubility of precipitated products encapsulated in solid matrices may result in resistance to reoxidation and leaching of TcO_4^-, synthetic approaches are also being formulated for the generation of solubility-limited technetium complexes by either sol-gel condensation or precipitation routes. In particular, we have devised routes for the synthesis of alkoxide complexes (which may be useful in protonation reactions designed to generate precipitated products), and will examine the base-induced condensation of technetium and rhenium complexes of the formula $MO_3(OSiMe_3)$ to generate the dimeric heptoxides $M_2O_7L_2$ (L = Lewis base).

Understanding the fundamental solution chemistry of Technetium materials is important for long-term storage concerns and the development of appropriate waste forms. The data derived from the investigation of Tc chemistry in its various oxidation states will provide the information needed for pretreatment schemes, processing, and the assessment of Tc stability in waste form materials.

Potential STCG Needs addressed

Mixed Waste Focus Area		
Field Office	**STCG Number**	**STCG Title**
SR	SR99-2049-S	Technetium Chemistry Under Waste Removal Conditions
Tanks Focus Area		
Field Office	**STCG Number**	**STCG Title**
RL	RL-WT033-S	Chemistry of Problem Constituents for HLW Virtrication
RL	RL-WT041-S	Radionuclide Partitioning

EMSP Research
Lawrence Berkeley National Laboratory

Project Number:	60328	**Award Year:**	1997
Project Title:	High Frequency Electromagnetic Impedance Measurements for Characterization, Monitoring and Verification Efforts		
Researchers:	Ki Ha Lee, Lawrence Berkeley National Laboratory Alex Becker, University of California Berkeley Louise Pellerin, Lawrence Berkeley National Laboratory		
EM Problem Areas:	Subsurface Contaminants (primary) Decontamination and Decommissioning High Level Waste		
Science Categories/ SubCategories:	Geophysics / Subsurface Imaging		
URL:	http://www.doe.gov /html/em52/60328.htm		

Synopsis:
Research on a non-invasive method for accurately imaging the electrical conductivity and dielectric permeativity of the shallow subsurface (<= 5 m) using the plane wave impedance approach.

Objective is to develop and test a proof of concept impedance approach that will allow for detailed mapping of the shallow subsurface

Non-invasive, high-resolution imaging of the shallow subsurface is needed for delineation of buried waste, detection of unexploded ordinance, verification and monitoring of containment structures, and other environmental applications. Electromagnetic measurements at frequencies between 1 and 100 MHz are important for such applications, because the induction number of many targets is small due, and the ability to determine the dielectric permittivity in addition to electrical conductivity of the subsurface is possible. Earlier workers were successful in developing systems for detecting anomalous areas, but no quantifiable information was accurately determined. For high resolution imaging, accurate measurements are necessary so the field data can be mapped into the space of the subsurface parameters.

This research plans to develop high-frequency impedance (HFI) methodology utilizing a window of the electromagnetic (em) spectrum from 1.0 MHz to 100 MHz. This window, between GPR and low-frequency induction techniques, has not been used to non-invasively investigate the upper few meters of the ground for environmental applications. Modeling and physical parameter studies confirm that impedance measurements at this frequency band can yield high-resolution mapping of the electrical conductivity as well as the permittivity. The impedance method has an advantage in that it is free of source coupling, so that the ensuing analysis tends to be much simpler

The research plan consists of three tasks:

1) Development of high frequency field measurement techniques,
2) Plane wave impedance estimation, and
3) Data processing, analysis, and interpretation

These tasks are being be investigated in a three-phase approach, roughly corresponding to three years total. The proof-of-concept will be determined with off-the-shelf test instrumentation and commercially available components, and the theoretical methods for impedance estimation, survey design, and sensitivity analysis will be fully developed, during phase 1. The proof-of-concept will provide the specifications necessary for assembling a prototype system, using off-the-shelf components and a modest engineering effort, in phase 2. Phase 3 will include the development of a data analysis package and field testing of the prototype system in order to verify the concept and proper operational procedures in known, well-characterized environments.

Potential STCG Needs addressed

Subsurface Contaminants Focus Area		
Field Office	**STCG Number**	**STCG Title**
ID	ID-S.1.04	Real-time Field Instrumentation for Characterization and Monitoring Soils and Groundwater.
NV	NV18-9902-04S	Long-Term Monitoring of Upward and Downward Pathways in the Vadose Zone and Closure Caps
Tanks Focus Area		
Field Office	**STCG Number**	**STCG Title**
RL	RL-WT045-S	Vadose Zone Flow Simulation Topol Under Arid Conditions

Project Number:	60362	**Award Year:**	1997
Project Title:	Ion-Exchange Processes and Mechanisms in Glasses		
Researchers:	B. Peter McGrail, Pacific Northwest National Laboratory - Lead David K. Shuh, Lawrence Berkeley National Laboratory John G. Darab, Pacific Northwest National Laboratory Donald R. Baer, Pacific Northwest National Laboratory		
EM Problem Areas:	High Level Waste (primary) Mixed Waste		
Science Categories/ SubCategories:	Materials Science / Chemical and Structural Properties Of Storage Materials		
URL:	http://www.doe.gov /html/em52/60362.html		

Synopsis:

Research on ion-exchange processes and mechanisms in low-activity waste glass.

> The objective of this work is to develop an understanding of the processes and mechanisms controlling alkali ion exchange and to correlate the kinetics of the ion-exchange reaction with glass structural properties.

Recent performance assessment calculations of a disposal system at the Hanford Site in Washington State for low-activity waste glass show that a sodium ion exchange reaction can effectively increase the radionuclide release rate by over a factor of 1000. The susceptibility of the glass to alkali ion exchange is thus a major factor limiting waste loading. However, low temperature ion exchange has not been investigated in recent analyses of waste glass durability.

Ion-exchange reaction mechanisms will be studied by using nuclear reaction analysis techniques to probe the distribution of isotopically-labeled elements in the hydrated layers on glass surfaces. Differences in the uptake and distribution of these isotopes will provide a signature characteristic of specific ion-exchange reactions. X-ray absorption spectroscopy will be used to identify and correlate key structural properties, such as the number of nonbridging oxygens, bonding of alkali to other elements in the glass, and alkali coordination, with differences in measured rates of alkali exchange. The Advanced Light Source (ALS) will be used to perform the measurements of actual waste glass data necessary to support the theoretical work.

The fundamental understanding of the ion-exchange process developed under this study will provide a sound scientific basis for formulating low exchange rate glasses with higher alkali waste loading, resulting in substantial production and disposal cost savings.

Potential STCG Needs Addressed

Tanks Focus Area		
Field Office	**STCG Number**	**STCG Title**
RL	RL-WT033-S	Chemistry of Problem Constituents for HLW Virtrication

EMSP Research
Lawrence Berkeley National Laboratory

Project Number:	60370	**Award Year:**	1997
Project Title:	Rational Design of Metal Ion Sequestering Agents		
Researchers:	Kenneth N. Raymond, Lawrence Berkeley National Laboratory		
EM Problem Areas:	Mixed Waste (primary) Decontamination and Decommissioning High Level Waste Nuclear Materials Subsurface Contaminants		
Science Categories/ SubCategories:	Actinide Chemistry / Actinide (Heavy Element) Chemistry (primary) Separations Chemistry / Ligand Design and Ion-exchange		
URL:	http://www.doe.gov /html/em52/60370.html http://www.homestead.com/knr/HomePage.html		

Synopsis:
Research on fundamental issues and requirements for developing hazardous metal ion (actinide) separation technologies needed for the treatment and disposal of radioactive and chemical toxic waste.

Objective is to develop new, metal ion specific complexing agents - very highly selective ligands that have high actinide affinity and selectivity.

Basic studies of the sequestration of relevant toxic metals are required in order to develop processes that will treat effluents sufficiently well to allow direct release into the environment and minimize the production of secondary wastes. Understanding the speciation and risks in nature from these hazardous metal ions requires the investigation of the thermodynamic data: coordination chemistry and stability of the metal complexes.

This research is focused on the following key areas:

1. Basic design and synthesis of new metal ion specific sequestering ligands;
2. Structural and thermodynamic investigations of these ligands and their complexes formed with the targeted metal ions; and
3. Development of sequestering agents and their incorporation into systems designed to be prototypes of inexpensive and highly effective materials for hazardous metal ion decontamination.

Research efforts for the first year were directed towards the thermodynamic characterization of the extraction agents and polymer-based materials with HOPO ligands which have shown great promise as Pu(IV) sequestering agents (fast kinetics, stability in acidic and alkaline conditions, and high affinity for Pu(IV) in the presence of EDTA or Fe(III) in large excess). Another route of investigation will be the thermodynamic characterization of uranyl complexes of HOPO and catecholamide ligands, since the uranyl ion has very different coordination chemistry from that of Pu(IV). In the second year of this project, the plan is to synthesize new liquid-liquid and polymer-supported extractants with improved properties and simplified preparation, based on our better understanding of their chemistry as a result of our studies.

These basic studies involving the investigation of the development of new, toxic metal ion complexing agents, should provide the information necessary to develop separation processes for the treatment and disposal of radioactive and chemical waste.

Potential STCG Needs addressed

Deactivation & Decommissioning Focus Area		
Field Office	**STCG Number**	**STCG Title**
RF	RF-DD09	Decontamination of Porous Surfaces
RF	RF-DD10	Decontamination Of Non-Porous Surfaces
RL	RL-DD026-S	Contaminant Binding Science Need

Project Number:	60387	**Award Year:**	1997

Project Title: Distribution & Solubility of Radionuclides & Neutron Absorbers in Waste Forms for Disposition of Plutonium Ash & Scraps, Excess Plutonium, and Miscellaneous Spent Nuclear Fuels

Researchers:
Xiangdong Feng, Pacific Northwest National Laboratory - Lead
Eric R. Vance, Australian Nuclear Science & Technology Organisation
David K. Shuh, Lawrence Berkeley National Laboratory
Rodney C. Ewing, University of Michigan
Hong Li, Pacific Northwest National Laboratory
Denis M. Strachan, Pacific Northwest National Laboratory
B. C. Bunker, Pacific Northwest National Laboratory
J. G. Darab, Pacific Northwest National Laboratory
M. J. Schweiger, Pacific Northwest National Laboratory
L. L. Davis, Pacific Northwest National Laboratory
L. Li, Pacific Northwest National Laboratory
J. D. Vienna, Pacific Northwest National Laboratory
P. G. Allen, Lawrence Berkeley National Laboratory
J. J. Bucher, Lawrence Berkeley National Laboratory
I. M. Craig, Lawrence Berkeley National Laboratory
N. M. Edelstein, Lawrence Berkeley National Laboratory
L. M. Wang, University of Michigan

EM Problem Areas: Nuclear Materials (primary)
Spent Nuclear Fuel

Science Categories/ SubCategories: Materials Science / Chemical and Structural Properties Of Storage Materials

URL: http://www.doe.gov /html/em52/60387.html

Synopsis:
Research on the effect of actinide oxidation states on its solubility in borosilicate based glasses.

The objective of this research is to gain a fundamental understanding of the distributions and the solubility limits for actinides and rare earth neutron absorbers in waste forms.

The objective of this research is to gain a fundamental understanding of the distributions and the solubility limits for actinides Pu and U and rare earth neutron absorbers such as Gd and Hf in waste forms. This will be accomplished by systematically studying the local structural environments of these constituents in representative waste forms such as glass, ceramics, and vitreous ceramics. The elucidation of the correlations between the local structural environments of actinides and rare earth neutron absorbers in waste forms as functions of waste form compositions, and waste form processing conditions will also advance basic material science.

The scope of this project includes the following:

1) A systematic investigation of the solubility and partition behavior of selected waste forms as a function of composition, temperature, and processing conditions with the goal of enhancing our understanding of the physics and chemistry of radionuclides and neutron absorbers in simplified waste forms;

2) Determination of the local structure of radionuclides and neutron absorbers waste forms in various phases:

    a) a microscale characterization to determine what phases are presented and how key elements are partitioned among those

    b) a molecular level characterization to understand local coordination

    c) an atomic level characterization to determine oxidation state

3) Selective study of waste form properties with the emphasis on the release behaviors of neutron absorbers and radionuclides.

Basic knowledge of these issues will provide a technical and scientific basis that can be used for developing, evaluating, selecting, and matching waste forms for the safe disposal of various wastes associated with Pu, miscellaneous spent nuclear fuels (SNF), and other transuranic (TRU) wastes and for developing deterministic model for the long-term performance assessment of radionuclide containment.

Potential STCG Needs addressed

Field Office	**STCG Number**	**STCG Title**
		None identified at this time.

EMSP Research
Lawrence Berkeley National Laboratory

Project Number: 60451 **Award Year:** 1997

Project Title: Mechanics of Bubbles in Sludges and Slurries

Researchers:
Phillip A. Gauglitz, Pacific Northwest National Laboratory - Lead
Morton M. Denn, Lawrence Berkeley National Laboratory
Susan J. Muller, Lawrence Berkeley National Laboratory
Guillermo Terrones, Pacific Northwest National Laboratory
William R. Rossen, University of Texas at Austin

EM Problem Areas: High Level Waste

Science Categories/ SubCategories: Engineering Science / Bubble Mechanics and Sonification

URL: http://www.doe.gov /html/em52/60451.html

Synopsis:
Research on the interactions between gas bubbles in high-level tank waste sludges and slurries.

The objective of this research project is to gain a fundamental understanding of the interactions between gas bubbles and tank waste sludges and slurries during barometric pressure fluctuations.

Previous studies have established that the waste level of Hanford tanks responds to barometric pressure changes, the compressibility of retained bubbles accounts for the level changes, and the volume of retained gas can be determined from the measured waste level and barometric pressure changes. However, interactions between the gas bubbles and rheologically complex waste cause inaccurate retained gas estimates and are not well understood. Because the retained gas is typically a flammable mixture of hydrogen, ammonia, and nitrous oxide, accurate determination of the retained gas volume is a critical component for establishing the safety hazard of the tanks. Accurate estimates of retained gas from level/pressure data are highly desirable because direct in situ measurements are very expensive in an individual tank and impossible in many single-shell tanks.

Th research on the modeling of the bubble/waste interactions is divided into four related problems comprising both theoretical and experimental studies.

1. Solid mechanics approach to modeling of the bubble/waste interactions - initiated with a theoretical study to understand the effects that smooth external pressure fluctuations have on the deformation history of a single bubble imbedded in a compressible elastic-perfectly plastic isotropic medium of infinite extent.
2. Continuum modeling from the fluid mechanics viewpoint - the interaction and movement of arrays of bubbles involve a number of scientific issues relating to flows of fluids exhibiting a yield stress.
3. For the modeling studies of bubbles in particulate materials (slurries), the pore structure is modeled as a one-dimensional (1-D) network of identical biconical pores with both converging and diverging sections.
4. For the experimental studies, the initial focus is to quantify the effect of small pressure changes on the volume of a single bubble in a waste simulant.

It is expected that the elucidation of the bubble/waste interaction mechanisms will lead to the development of models for a more accurate determination of: gas content in Hanford tanks, waste properties from level/pressure data, and the effect that barometric pressure fluctuations have on the slow release of bubbles.

Potential STCG Needs addressed

Tanks Focus Area		
Field Office	**STCG Number**	**STCG Title**
RL	RL-WT042-S	Flammable Gas Generation, Retention, and Release in HLW Tanks
RL	RL-WT051-S	Foam Generation and Stability

EMSP Research
Lawrence Berkeley National Laboratory

Project Number:	65015	**Award Year:**	1998
Project Title:	Three-Dimensional Position-Sensitive Germanium Detectors		
Researchers:	Mark Amman, Lawrence Berkeley National Laboratory - Lead Paul N. Luke, Lawrence Berkeley National Laboratory		
EM Problem Areas:	Decontamination and Decommissioning		
Science Categories/ SubCategories:	Engineering Science / Diagnostics		
URL:	http://www.doe.gov /html/em52/65015.html		

Synopsis:
Research to develop three-dimensional position-sensitive germanium detectors with the ultimate goal of improving image resolution without sacrificing spectroscopic resolution in gamma-ray imaging cameras.

The objective of this research is the focus on the radioactive materials characterization needs of DOE's decontamination and decommissioning effort.

Gamma-ray imaging and spectroscopy together form a potentially powerful tool for the passive, non-destructive and non-intrusive identification and spatial mapping of contaminated structures. Germanium position-sensitive gamma-ray detectors offer the advantages of excellent energy resolution required for clear isotopic identification combined with potentially high spatial resolution. With the addition of depth-of-interaction sensing to conventional two-dimensional position-sensitive detectors, we will be able to greatly reduce the image degradation effects caused by Compton scattering and parallax, thereby increasing the resolving power of the detectors.

The goals of this research include following:

- In-situ identification, spatial mapping, and quantification of contaminants;
- Improved image resolution in germanium-based detectors for gamma ray imaging;
- Quick and accurate characterization of radioactively contaminated equipment and structures;
- Methods to improve image resolution in germanium-based ray detectors;
- Detector physics and fabrication technology of high-spatial-resolution germanium detectors

The technical approach for this research

1. More accurately locate the -ray interaction events in the detector by measuring the interaction location in all three dimensions rather than just two
2. Develop detectors based on LBNL technologies with the simplest possible electrode structures to reduce system complexity and difficulties in fabrication.

The technology developed from this research will form the basis for the design and fabrication of future high-performance gamma-ray imaging cameras

Potential STCG Needs Addressed

Deactivation & Decommissioning Focus Area		
Field Office	**STCG Number**	**STCG Title**
RL	RL-DD023-S	Cesuim Source Identification
Mixed Waste Focus Area		
Field Office	**STCG Number**	**STCG Title**
AL	AL-09-01-24-MW-S	Radioassay of Remote-Handled Transuranic (RH-TRU) Waste Containers to Meet WIPP Data Quality
AL	AL-09-01-25-MW-S	Radioassay of Very Large Containers of Low-Level Contact-Handled Transuranic (CH-TRU) Waste to Meet WIPP Data Quality Assurance Objectives
ID	ID-S.1.05	Nondestructive Assay (NDA) Capability for Remote-Handled Transuranic Waste
ID	ID-S.2.02	Nondestructive Assay (NDA) for Resource Conservation and Recovery Act Metal and Chlorine in Incinerator Feed
ID	None	NDA for RCRA and Cl in drums, boxes, and mics. Debris
ID	None	NDA for TRU in drums, boxes, and mics. Debris
Nuclear Materials Focus Area		
Field Office	**STCG Number**	**STCG Title**
RF	RF-WM04	Improved Sensitivity For Plutonium Assay Instrumentation
RF	RF-WM04-98	Improved Sensitivity For Plutonium Non-Destructive Assay (NDA) Instrumentation
Subsurface Contaminants Focus Area		
Field Office	**STCG Number**	**STCG Title**
ID	ID-6.1.01	In-Situ Debris Characterization for Partial Retrieval

EMSP Research
Lawrence Berkeley National Laboratory

Project Number: 65352 **Award Year:** 1998

Project Title: Developing a Fundamental Basis for the Characterization, Separation, and Disposal of Plutonium and other Actinides in High Level Radioactive Waste: The Effect of Temperature and Electrolyte Concentrations on Actinide Speciation

Researchers: Sue B. Clark, Washington State University - Lead
Linfeng Rao, Lawrence Berkeley National Laboratory
Scott Wood, University of Idaho

EM Problem Areas: High Level Waste
Science Categories/ SubCategories: Actinide Chemistry / Actinide (Heavy Element) Chemistry

URL: http://www.doe.gov /html/em52/65352.html

Synopsis:
Research on developing a scientific basis for describing the speciation of the actinides and Pu in high level radioactive waste (HLW).

This objective of this research is to experimentally derive a thermodynamic model of Pu/actinide complexation under chemically harsh conditions relevant to HLW.

While DOE has supported research on Pu speciation in acidic systems as needed for separations processing during the Cold War, or in concentrated electrolytes to support Pu disposal in the Waste Isolation Pilot Plant (WIPP), application of the results from such programs to predict the speciation of Pu in HLW is not adequate. Chemical equilibria are dependent on system conditions. Conditions relevant to HLW include highly alkaline aqueous systems with extremes in electrolyte concentrations (e.g., 5 molal and greater), and elevated temperatures (e.g., T = 300°C is possible in the HLW repository)

This research plans to develop a scientific basis for describing the speciation of the actinides and Pu in such systems. This basis will consist of an experimentally-derived thermodynamic model of Pu/actinide complexation under chemically harsh conditions relevant to HLW. The research plan is to systematically measure the effects of pH, electrolyte concentrations, and temperature on Pu and actinide solution chemistry in a Na-NO_3-OH-H_2O matrix. Both chemical analogs of the different oxidation states of Pu (e.g., Nd^{3+}, Th^{4+}, NpO_2^{2+}, and UO_2^{2+}) and Pu itself will be studied. They will determine

- the temperature dependence of ion interaction parameters for these cations with NO_3^-
- will study their complexation behavior with OH^-, acetate, oxalate, and EDTA.

The experimental plan combines several approaches intended to define the underlying molecular processes responsible for the electrolyte and temperature dependence of actinide complexation equilibria. Stability constants, enthalpies and entropies for complexation will be determined under alkaline conditions, and at variable ionic strengths and temperatures. In addition, spectroscopic tools will be used to directly observe changes in metal hydration for the complexes formed. Correlations between the temperature and ionic strength dependence of the primary hydration sphere and the observed stability constants will be used to elucidate the role of water in actinide complexation in such extreme conditions. Understanding the role of water is an important parameter for developing a predictive model applicable to the myriad of possible actinide complexation reactions in HLW from a limited experimental data set.

Using the experimental results for the systems outlined above, a Pitzer model will be build to describe the speciation of Pu and the actinides in alkaline conditions as a function of elevated ionic strengths and temperatures. The modeling efforts will be an extension of existing DOE research describing the temperature dependence of the electrolyte matrix for the Hanford waste tanks. The "actinide specific" information will be added to the temperature dependence Pitzer model for HLW. The model predictions will be validated by comparison to observed actinide and Pu speciation in actual HLW.

With the temperature dependence Pitzer model for Pu and the other actinides developed from this research program, DOE will be able to predict the speciation of Pu and the actinides over all ranges of temperatures and ionic strengths relevant to characterization, pretreatment and separation, and disposal of HLW. In addition, prediction of the conditions necessary to favor the formation of a desired chemical form will also be possible. With such a powerful predictive tool, the successful development of cost-effective technologies necessary to remediate the HLW tanks becomes much more probable.

Potential STCG Needs Addressed

Nuclear Materials Focus Area		
Field Office	**STCG Number**	**STCG Title**
AL	AL-09-01-23-Pu-S	Selective Aqueous Non-invasive Extractions of Low and Medium Fired PuO2 from High Level Wastes, Residues, and Concentrates
Tanks Focus Area		
Field Office	**STCG Number**	**STCG Title**
RL	RL-WT041-S	Radionuclide Partitioning
RL	RL-WT048-S	Innovative Methods for Radionuclide Separation
RL	RL-WT049-S	Effect of Processing on Waste Rheological and Sedimentation Properties

EMSP Research
Lawrence Berkeley National Laboratory

Project Number: 65368 **Award Year:** 1998

Project Title: Speciation, Dissolution, and Redox Reactions of Chromium Relevant to Pretreatment and Separation of High-Level Tank Wastes

Researchers: Linfeng Rao, Lawrence Berkeley National Laboratory - Lead
Dhanpat Rai, Pacific Northwest National Laboratory
Sue B. Clark, Washington State University

EM Problem Areas: High Level Waste

Science Categories/ SubCategories: Separations Chemistry / Ligand Design and Ion-exchange

URL: http://www.doe.gov /html/em52/65368.html

Synopsis:
Research seeking fundamental knowledge of Cr chemistry in multi-component, highly non-ideal electrolyte systems.

> The objective is to provide critical data to support the development of pretreatment processes for the removal of Cr from HLW tank sludge.

Chromium (Cr), one of the problematic constituents in tank sludges, is presently considered to be the most important constituent in defining the total volume of HLW glass to be produced from the Hanford tank wastes, because it greatly complicates the vitrification process by forming separate phases in the molten glass and, more importantly, current sludge washing processes are not effective in the removal of chromium from sludges could result in production of an unacceptably large volume of HLW glass.

The removal of Cr from tank sludges is complicated by factors including the complex chemistry of Cr, lack of fundamental data applicable to the HLW chemical systems (high heterogeneity, high ionic strength, high alkalinity and presence of inorganic and organic ligands, etc.), and the need to avoid processes that may adversely enhance the solubility of Pu and other actinides. Significant gaps exist in the fundamental understanding of Cr chemistry in tank-like environments. Without such understanding, these strategies cannot be appropriately evaluated or optimized.

Using an integrated approach of solubility measurements and spectroscopic characterization to study the speciation, dissolution and redox reactions of Cr under conditions relevant to HLW processing.

- Solubilities and dissolution rates of important Cr compounds will be determined as functions of ionic strength, alkalinity, redox conditions and temperature.
- Dominant Cr species in both solution and solid phases under these conditions will be characterized.
- A model will be developed and tested describing the dissolution/precipitation behavior of Cr under HLW processing conditions with controlled HLW sludge leaching tests.

This research should provide data critical to support the development of pretreatment processes for the removal of Cr and thereby helping to achieve a major saving in the cost of HLW disposal.

Potential STCG Needs Addressed

Tanks Focus Area		
Field Office	**STCG Number**	**STCG Title**
RL	RL-WT048-S	Innovative Methods for Radionuclide Separation
RL	RL-WT049-S	Effect of Processing on Waste Rheological and Sedimentation Properties

EMSP Research
Lawrence Berkeley National Laboratory

Project Number:	65370	**Award Year:**	1998
Project Title:	Actinide-Specific Interfacial Chemistry of Monolayer Coated Mesoporous Ceramics		
Researchers:	Glen E. Fryxell, Pacific Northwest National Laboratory - Lead Ken Kemner, Argonne National Laboratory K.N. Raymond, Lawrence Berkeley National Laboratory		
EM Problem Areas:	High Level Waste		
Science Categories/ SubCategories:	Actinide Chemistry / Actinide (Heavy Element) Chemistry		
URL:	http://www.doe.gov /html/em52/65370.html		

Synopsis:
Research aimed at understanding and optimizing the actinide-specific interfacial chemistry of monolayer coated mesoporous ceramics

The objective is to build on the SAMMS (self-assembled monolayers on mesoporous supports) design and concept and extend the interfacial chemistry of monolayer coated mesoporous materials to study the requirements of selective binding of actinides.

The need exists in the management of Hanford's high level wastes (HLW) to be able to selectively and completely remove the actinides so that HLW volume can be minimized and the nonradioactive components can be segregated and disposed of as low level waste. In addition, the short-term risk assessment for tank closure requires a complete and accurate accounting of actinide speciation. These needs dictate the development of selective and efficient separation of actinides from complex waste streams so as to minimize HLW volume, reduce waste management costs and enhance long-term stability of the HLW form. PNNL has developed (SAMMS) as a superior method of mercury and heavy metal sequestration. SAMMS has proven to be orders of magnitude faster and more effective than existing mercury scavenging methods.

A multi-faceted study will be used for this research:

1. Explore and develop novel mesoporous synthetic strategies utilizing non-ionic surfactants. Some of these novel mesoporous materials are anticipated to have beneficial properties as actinide sorbent supports due to their neutron scavenging capabilities.

2. Study the use of supercritical fluids for the deposition of self-assembled monolayers in mesoporous ceramics to increase reaction efficiency, reaction rate, molecular order, loading density, and purity of the final SAMMS product.

3. Study the efficiency and selectivity of these interfacial ligand fields for actinide separations once these molecules are anchored to the monolayer interface.

The integrated results from these design, synthesis, characterization and sorption studies are key for the successful design and construction of efficient actinide sorbent materials.

Potential STCG Needs Addressed

Tanks Focus Area		
Field Office	**STCG Number**	**STCG Title**
RL	RL-WT048-S	Innovative Methods for Radionuclide Separation

EMSP Research
Lawrence Berkeley National Laboratory

Project Number:	65398	**Award Year:**	1998
Project Title:	Characterization of Actinides in Simulated Alkaline Tank Waste Sludges and Leach Solutions		
Researchers:	Kenneth L. Nash, Argonne National Laboratory - Lead Linfeng Rao, Lawrence Berkeley National Laboratory		
EM Problem Areas:	High Level Waste		
Science Categories/ SubCategories:	Actinide Chemistry / Actinide (Heavy Element) Chemistry		
URL:	http://www.doe.gov /html/em52/65398.html		

Synopsis:
Research designed to provide new fundamental information on the chemical behavior and speciation of uranium, neptunium, plutonium, and americium in simulated alkaline tank waste sludges and alkaline scrub liquors.

> The objective of this research is to provide new information that will increase predictability of actinide behavior during waste tank remediation, and so contribute to minimization of the volume of high level waste created.

The expectation that solubility of actinide ions will be low during alkaline sludge washing to remediate DOE's underground waste tanks is based on minimal experimental evidence, and the application of thermodynamic models of dubious validity to systems that may well be under kinetic control. There are essentially no data describing the chemical speciation of actinides in waste tank sludges.

Sludges representative of those generated during plutonium production will be prepared using appropriate combinations of chemical components of the various waste streams that contribute to the complexity of alkaline tank wastes. Actinide ions will be introduced in the oxidation states pertinent to process conditions at concentrations ranging from nil to macroscopic. Actinide speciation in the insoluble sludges will be examined using X-ray diffraction and other scattering techniques.

Parallel studies will address the chemistry of actinide ions in alkaline solutions, principally those containing chelating agents. By correlating actinide speciation in the solid and solution phases with sludge composition, it will be possible to predict conditions favoring mobilization (or immobilization) of actinide ions during sludge washing.

Potential STCG Needs Addressed

Tanks Focus Area		
Field Office	**STCG Number**	**STCG Title**
RL	RL-WT041-S	Radionuclide Partitioning

Section 3:

Current Lawrence Livermore National Laboratory EMSP projects

EMSP Research
Lawrence Livermore National Laboratory

Project Number:	54576	**Award Year:**	1996
Project Title:	On the Inclusion of the Interfacial Area Between Phases in the Physical and Mathematical Description of Subsurface Multiphase Flow		
Researchers:	William G. Gray, University of Notre Dame – Lead Andrew ‘Andy’ Tompson, Lawrence Livermore National Laboratory Wendy E. Soll, Los Alamos National Laboratory		
EM Problem Areas:	Subsurface Contaminants		
Science Categories/ SubCategories:	Hydrogeology / Instrumentation and Modelling		
URL:	http://www.doe.gov /html/em52/54576.html		

Synopsis:
Research to improve modeling prediction of contaminant movement through the subsurface.

> The objective of this research is to achieve better modeling of subsurface multiphase flow through inclusion of fluid-fluid interface in porous media

A distinguishing feature of multiphase subsurface flow in comparison to single phase flow is the existence of fluid-fluid interfaces. These interfaces define phase boundaries at the pore scale and influence overall system behavior in many important ways. For example, fluid-fluid interfaces support non-zero stresses, allowing for different phase pressures across each interface. In problems of inter-phase mass transfer, such as evaporation in air-water systems or dissolution in hydrocarbon-water systems, all mass is exchanged via the interfaces. While interfaces are central to multi-phase flow physics and associated contaminant transport, their treatment in traditional porous-media theories has been given little attention. Recent theoretical work provides a general framework within which interfacial area is incorporated explicitly into volume-averaged equations for conservation of mass, momentum, and energy. This leads to an expanded set of continuum-scale equations that carry the overhead burden of the associated set of expanded constitutive relationships. To make these equations a scientifically useful tool for the study of the soil environment, parameterization of the constitutive forms must occur. This parameterization requires that the equations be studied in light of the actual behavior of porous media systems. To perform the early stages of this work effectively, the porous media must be controlled, well-understood systems that lend themselves to careful scientific analysis.

This project implements a three-pronged approach to assessing the importance of various features of multiphase flow to its description. This research aims to contribute to the improved understanding and precise physical description of multiphase subsurface flow by combining

1. theoretical derivation of equations,
2. lattice Boltzmann modeling of hydrodynamics to identify characteristics, and
3. solution of the field-scale equations using a discrete numerical method to assess the advantages and disadvantages of the complete theory.

This approach includes both fundamental scientific inquiry and a path for inclusion of the scientific results obtained in a technical tool (model) that will improve assessment capabilities for multiphase flow situations that have arisen due to spills of organic materials in the natural environment.

Potential STCG Needs Addressed

Subsurface Contaminants Focus Area		
Field Office	**STCG Number**	**STCG Title**
AL	AL-09-01-08-SC-S	Differences Between Saturated and Unsaturated Systems
ID	ID-S.2.03	Aqueous Transport of Soluble Radionuclides and Heavy Metals: Evaluation of Non-Equilibrium Processes and Native Surfaces in Porous Media
RL	RL-SS31-S	Mathematical Formulations of Chemical Reaction/Material Transport

EMSP Research
Lawrence Livermore National Laboratory

Project Number:	54950	**Award Year:**	1996
Project Title:	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes		
Researchers:	Charles R. Carrigan, Lawrence Livermore National Laboratory - Lead G. Bryant Hudson, Lawrence Livermore National Laboratory		
EM Problem Areas:	Subsurface Contaminants		
Science Categories/ SubCategories:	Hydrogeology / Instrumentation and Modelling		
URL:	http://www.doe.gov /html/em52/54950.html		

Synopsis:
Research to obtain improved understanding of vadose zone transport processes and to develop field and modeling techniques required to characterize contaminant transport in the unsaturated zone at DOE sites.

The objective of this research is to provide a new methodology or way of thinking about vadose zone characterization and modeling from a site specific perspective. This will aid in helping to dynamically characterize vadose zones at a site.

For surface spills and near-surface leaks of chemicals, the vadose zone may well become a long-term source of contamination for the underlying water table. Transport of contaminants can occur in both the liquid and gas phases of the unsaturated zone. This transport occurs naturally as a result of diffusion, buoyancy forces (gravity), capillarity and barometric pressure variations. In some cases transport can be enhanced by anisotropies present in hydrologic regimes. This is particularly true for gas-phase transport which may be subject to vertical pumping resulting from atmospheric pressure changes. For liquid-phase flows, heterogeneity may enhance the downward transport of contaminants to the water table depending on soil properties and the scale of the surface spill or near-surface leak. Characterization techniques based upon the dynamics of transport processes are likely to yield a better understanding of the potential for contaminant transport at a specific site than methods depending solely on hydrologic properties derived from a borehole.

As discussed above, complex interactions between the atmosphere and groundwater can take place in the vadose zone. Several stages in the transport process are involved in going from a volatile, liquid state contaminant to a contaminant vapor vented at the surface. The Vadose Zone Transport Study is investigating the detailed nature of each of these stages of transport in several different kinds of vadose regimes in the following manner:

- using existing data,
- new field studies involving dissolved tracer gases, and
- 3-D diagnostic computer simulations that provide a framework to interpret the observations.

The research is emphasizing the impact of features specific to a site, i.e., the local geology and hydrology, on each stage of the transport process. In particular, the researchers want to better understand how the specific character of a site impacts the time scales for

(1) partitioning contaminants from the liquid to the vapor states, and

(2) transporting the vapor out of the vadose regime.

Such time-scale information will be important for evaluating the potential of contaminant sources as well as remediation strategies including natural remediation approaches.

The dynamic-characterization techniques being investigated in this research project have the potential for being useful for evaluating sites where contamination presently exists as well as for providing an objective basis to evaluate the efficacy of proposed as well as implemented clean-up technologies. The real-time monitoring of processes that may occur during clean-up of tank waste and the mobility of contaminants beneath the Hanford storage tanks during sluicing operations is one example of how techniques developed in this effort can be applied to current remediation problems. In the future, such dynamic-characterization methods might also be used as part of the site-characterization process for determining suitable locations of new facilities that have the potential of introducing contamination into the vadose zone.

Potential STCG Needs Addressed

Subsurface Contaminants Focus Area		
Field Office	**STCG Number**	**STCG Title**
AL	AL-09-01-03-SC-S	Succession and Long-Term Performance of Landfill Covers
AL	AL-09-01-06-SC-S	Issue of Scale in Flow Prediction and Contaminant Remediation in Porous Media
AL	AL-09-01-08-SC-S	Differences Between Saturated and Unsaturated Systems
AL	AL-09-01-10-SC-S	Physics of Fracture Flow and Transport in the Vadose Zone
AL	AL-09-01-11-SC-S	Water Fluxes and Solute Transport in Arid and Semiarid Environments
AL	AL-09-01-12-SC-S	Groundwater-Surface Water Interactions
AL	AL-09-01-14-SC-S	Vadose Zone Flux Rates
ID	ID-S.1.04	Real-time Field Instrumentation for Characterization and Monitoring Soils and Groundwater.
ID	ID-S.1.07	Facilitated Transport at DOE Disposal Sites
ID	ID-S.1.08	Contaminant Transport in a Fractured Rock Vadose Zone
NV	NV18-9902-04S	Long-Term Monitoring of Upward and Downward Pathways in the Vadose Zone and Closure Caps
OK	OK99-20	Innovative Technology to Investigate Geology and Groundwater Flow Characteristics in Fractured Rock
OR	ORHY-01a	Dense Non-Aqueous Phase Liquid (DNAPL) Source Characterization, Containment, and Treatment
OR	ORHY-12a	Active In Situ Dissolved Phase Treatment Systems
RL	RL-SS26-S	Reaction Rates for Key Contaminant Species and Complexes in Site-Specific

		Groundwaters
RL	RL-SS29-S	Effect of Subsurface Heterogeneities on Chemical Reaction and Transport

Tanks Focus Area		
Field Office	**STCG Number**	**STCG Title**
RL	RL-WT035-S	Moisture Flow and Contaminant Transport in Arid Conditions
RL	RL-WT045-S	Vadose Zone Flow Simulation Topol Under Arid Conditions
RL	RL-WT053-S	Containment Mobility Beneath Tank Farms

EMSP Research
Lawrence Livermore National Laboratory

Project Number: 55011 **Award Year:** 1996

Project Title: Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes

Researchers: James G. Berryman, Lawrence Livermore National Laboratory

EM Problem Areas: Subsurface Contaminants

Science Categories/ SubCategories: Geophysics / Subsurface Imaging

URL: http://www.doe.gov /html/em52/55011.html

Synopsis:

Research on the use of magnetic fields to image conductors in the subsurface: Electromagnetic Induction Tomography (EMIT)

> The objective of this project is to produce enhanced images of electrically conducting fluids underground.

Electromagnetic induction logging has long been used in the petroleum and environmental business to measure the electrical conductivity in the region immediately surrounding the borehole. This data, which is used to estimate pore fluid saturations near the well, is very sensitive to variations in rock pore fluid. Mapping surface variation of conductivity has also been found to be a very sensitive indicator of zones of higher salinity and acidity in many shallow environmental studies.

While other technologies such as Electrical Resistance Tomography (ERT) can produce electrical conductivity images at a useful spatial scale, the advantage of the electromagnetic induction technology is that it can make use of existing monitoring wells and the surface to do imaging. Since signals are transmitted and received inductively, it is not necessary to make ground contact (no ground penetrating electrodes); the technology is therefore relatively noninvasive. There is also the important potential advantage that multiple frequencies can be employed to improve the imaging capability for electromagnetic induction tomography; this feature is not available with ERT imaging since the inversion methods used are inherently based on the DC (zero frequency) limit of the pertinent equations.

Although field techniques have been developed and applied to collection of such EM data, the algorithms for inverting the magnetic data to produce the desired images of electrical conductivity have not kept pace. The current state of the art in electromagnetic data inversion is based on the Born/Rytov approximation (requiring a low contrast assumption), or extensions. However, it is known that conductivity variations in fact range over several orders of magnitude and therefore require nonlinear analysis. The goal of this project is therefore to join theory and experiment to produce enhanced images of electrically conducting fluids underground, allowing better localization of contaminants and improved planning strategies for the subsequent remediation efforts.

To achieve this goal, the research is pursuing the following tracks:

- development and improvements to the field data acquisition system
- development of an inversion code to analyze the data

The development of this technology will allow for the determination of subsurface conductivity at a much higher resolution than can be achieved with surface techniques and much greater penetration than can be achieved with radar technology.

Potential STCG Needs Addressed

Subsurface Contaminants Focus Area		
Field Office	**STCG Number**	**STCG Title**
AL	AL-09-01-03-SC-S	Succession and Long-Term Performance of Landfill Covers
ID	ID-S.1.04	Real-time Field Instrumentation for Characterization and Monitoring Soils and Groundwater.
ID	ID-S.2.01	Definition of ´Biologically Active Zones´ in Fractured Rock Environments
NV	NV18-9902-04S	Long-Term Monitoring of Upward and Downward Pathways in the Vadose Zone and Closure Caps
OK	OK99-20	Innovative Technology to Investigate Geology and Groundwater Flow Characteristics in Fractured Rock
OR	ORHY-01a	Dense Non-Aqueous Phase Liquid (DNAPL) Source Characterization, Containment, and Treatment
RL	RL-SS25-S	Chemical Form and Mobility of Dense, Non-Aqueous Phase Liquids in Hanford Subsurface Transport of Contaminants

EMSP Research
Lawrence Livermore National Laboratory

Project Number:	55148	**Award Year:**	1996

Project Title: Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry

Researchers: Gregory Nimz, Lawrence Livermore National Laboratory - Lead
Marc Caffee, Lawrence Livermore National Laboratory
Robert Finkel, Lawrence Livermore National Laboratory
Jeffrey McAninch, Lawrence Livermore National Laboratory

EM Problem Areas: Subsurface Contaminants (primary)
High Level Waste

Science Categories/ SubCategories: Geochemistry / Sorption/Desorption

URL: http://www.doe.gov /html/em52/55148.html

Synopsis:
Research to develop techniques for measuring globally distributed radionuclides occurring in extremely low abundances and applying these techniques to better understand the mechanisms by which radionuclides migrate in the subsurface.

> Objective is to identify and quantify the geochemical parameters controlling the migration of key radionuclides (^{36}Cl, ^{90}Sr, ^{93}Zr, ^{99}Tc and ^{129}I) in undisturbed soils of the shallow and deep vadose zone.

The current scientific understanding of the geochemical parameters controlling the migration of radionuclides cannot sufficiently meet the requirements for at least two determinations necessary for environmental management in the United States: moisture flux through unsaturated soils, and contaminant radionuclide migration in the far-field environment. This research will perform radionuclide measurements using newly developed techniques employing accelerator mass spectrometry (AMS), which provides the required analytical sensitivity such that this work can be conducted for the first time.

The investigations in the shallow-zone, where the relationship between nuclide concentration and soil characteristics (composition, texture) can be identified, are expected to greatly improve our understanding of the relationship between chlorine-^{36}Cl distribution and moisture flux. The work on the deep-zone, and the resulting numerical model, is expected to provide a much clearer understanding of the potential for radionuclide transport far away from the contaminant release point, in an environment that is otherwise natural and undisturbed (i.e., in the far-field environment). The radionuclides targeted in this study were distributed globally during the era of atmospheric nuclear testing, and occur in virtually all geological and biological environments. The development of ultrasensitive AMS techniques for their detection in small samples will provide the means to assess radionuclide migration in most of these environments. This will result in a far greater understanding of potential health risks in the far-field environment, where the public is most likely to come into contact with contaminants. The targeted radionuclides are not only themselves common contaminants, but also are representative of classes of radionuclides and heavy metals that exhibit similar migration behavior. The models developed in this research will therefore furnish a foundation for a wide variety of contaminant migration assessments.

The advantages of this approach include the following: 1) the ability to conduct migration studies in locations most like those of concern to public health, e.g., a “far-field” environment; 2) sites of multiple contamination, e.g., by VOCs, can be avoided; 3) it becomes unnecessary to collect research samples that are themselves radioactive waste and are therefore difficult to handle and dispose of in the laboratory; and 4) since the nuclides are globally distributed, migration research can be conducted in any chosen environment.

The research is composed of the following components:

(1) develop AMS analytical methods for ^{90}Sr, ^{93}Zr, ^{99}Tc, ^{129}I;
(2) improve AMS ^{36}C1 and chlorine methods for determining moisture flux in arid soils;
(3) measure the distribution of ^{90}Sr, ^{93}Zr, ^{99}Tc, ^{129}I relative to the moisture flux in a vadose zone as defined by chloride and ^{36}C1 movement; and
(4) develop a numerical model simulating the migration which produced the observed distribution.

To date, the researchers have developed new technology for measuring/analyzing ^{99}Tc and ^{129}I and improved techniques for measuring ^{36}Cl using the new AMS analytical techniques. As discussed above these techniques have an advantage over current techniques in that they have no special specimen requirements. Subsequent work will use this data to take the measure the distribution of the selected radionuclides relative to the moisture flux in a vadose zone and develop a model the simulating the observed far field migration.

Potential STCG Needs Addressed

Subsurface Contaminants Focus Area		
Field Office	**STCG Number**	**STCG Title**
OR	ORHY-12a	Active In Situ Dissolved Phase Treatment Systems
Tanks Focus Area		
Field Office	**STCG Number**	**STCG Title**
RL	RL-WT046-S	Getter Materials
RL	RL-WT053-S	Containment Mobility Beneath Tank Farms

EMSP Research
Lawrence Livermore National Laboratory

Project Number:	55249	**Award Year:**	1996
Project Title:	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time and Solution Chemistry		
Researchers:	Susan Carroll, Lawrence Livermore National Laboratory – Lead Carol Bruton, Lawrence Livermore National Laboratory Peggy O'Day, Arizona State University Nita Sahai, Arizona State University		
EM Problem Areas:	Subsurface Contaminants		
Science Categories/ SubCategories:	Geochemistry / Sorption/Desorption		
URL:	http://www.doe.gov /html/em52/55249.htm		

Synopsis:
Research on the geochemical processes that control the mobility of Sr in the presence of clays (kaolinite, montmorillonite) and iron hydroxides (goethite) as a function of temperature, pH, and time.

> The objective of this work is to determine the fundamental data needed to predict the behavior of Sr at temperature and time scales appropriate to thermal remediation.

Strontium is significantly more mobile than other hazardous radioactive metals. Its partitioning between aqueous and solid phases is controlled by reactions that occur at the interface between natural waters and minerals. At a groundwater site in Hanford (200-BP-5), the aerial extent of the ^{90}Sr plume is 100 times larger than the aerial extent of the ^{137}Cs and the ^{239}Pu plumes. Similarly, contaminated, perched watertables at INEEL have much higher aqueous concentrations of ^{90}Sr than ^{137}Cs, presumably because Cs is preferentially sorbed to solids (Duncan 1995). Under high physical flow conditions, such as those in the highly fractured rock at Hanford and INEL, ^{90}Sr present in plumes may spread off-site and cause contamination of aquifers or other water sources. Geochemical factors that may contribute to the overall mobility of Sr in natural waters are the solubilities of phases such as strontianite ($SrCO_3$) and formation of strong complexes with sulfate and nitrate.

The research approach combines macroscopic sorption/precipitation and desorption/dissolution kinetic experiments, which track changes in solution composition, with direct molecular characterization of strontium in the solid phase using X-ray absorption spectroscopy. These experiments will be used to identify mechanistic geochemical reactions and their thermochemical properties that will be incorporated into geochemical computer codes to develop a model to predict Sr mobility.

The model developed by this research will be based on the mechanistic geochemical reactions and thermochemical properties identified in the experiments, such that this information can be used to predict ^{90}Sr mobility at Hanford and potential radioactive waste repositories, and to optimize any clean-up programs.

Potential STCG Needs Addressed

Subsurface Contaminants Focus Area		
Field Office	**STCG Number**	**STCG Title**
ID	ID-S.2.03	Aqueous Transport of Soluble Radionuclides and Heavy Metals: Evaluation of Non-Equilibrium Processes and Native Surfaces in Porous Media
OR	ORHY-12a	Active In Situ Dissolved Phase Treatment Systems

EMSP Research
Lawrence Livermore National Laboratory

Project Number: 55411 **Award Year:** 1996

Project Title: Joint Inversion of Geophysical Data for Site Characterization and Restoration Monitoring

Researchers: Patricia A. Berge, Lawrence Livermore National Laboratory – Lead
Jeffery J. Roberts, Lawrence Livermore National Laboratory
James G. Berryman, Lawrence Livermore National Laboratory
Dorthe Wildenschild, Lawrence Livermore National Laboratory

EM Problem Areas: Subsurface Contaminants (primary)
High Level Waste

Science Categories/ SubCategories: Geophysics / Subsurface Imaging

URL: http://www.doe.gov /html/em52/55411.html
http://www-ep.es.llnl.gov/www-ep/esd/expgeoph/Berge/EMSP/

Synopsis:
Research is focused on developing a code for joint inversion of seismic and electrical data, to improve underground imaging for site characterization and remediation monitoring.

> Objective of the research is to use geophysical and well-test data to provide accurate information about porosity, saturation, and permeability between wells.

Effective in-situ remediation requires knowledge of subsurface porosity, permeability, and fluid saturation. Only after the site has been characterized can the clean up begin. Using geophysical techniques to image the subsurface is much cheaper and less invasive than drilling many sampling wells. Electrical methods have usually been used for environmental applications, but recent advances in high-resolution crosswell seismic methods (e.g., Harris et al., 1995) suggest that combined electrical and seismic techniques could be a powerful tool for imaging the shallow subsurface.

Surface and borehole geophysical data have been used for a number of years for site characterization and clean-up monitoring (e.g., Ramirez et al., 1993, 1995; Wilt et al., 1995a,b) and monitoring steam-flooding in hydro-carbon reservoirs (e.g., Harris, 1988; Mathisen et al., 1995), but these data may only indirectly measure the site structure and fluid flow parameters that control the storage and movement of subsurface fluids. The current practice in geophysics is to interpret a single geophysical data set to obtain an image of a single geophysical parameter, such as seismic velocity or electrical resistivity. The geologic parameters of interest (i.e., the permeability, porosity, and fluid distribution) are usually estimated by overlaying a series of these geophysical images. Current estimation techniques are very subjective, and geologic parameters are not obtained directly. Current practices also do not exploit the complementary capabilities of seismic and electrical methods. Seismic methods are best for resolving subsurface structure and porosity (e.g., Lines et al., 1993; Mathisen et al., 1995), whereas electrical methods are preferred for identifying fluids, saturation, and permeability (e.g., Wilt et al., 1995a,b).

The goal of this project is to develop a code for joint inversion of seismic and electrical data. The new computer code developed in this project will invert geophysical (seismic) data to obtain direct estimates of porosity and saturation underground, rather than inverting for seismic velocity and electrical resistivity or other geophysical properties. This method exploits the complementary nature of seismic and electrical measurements, and leads to an objective estimate of the geological and fluid flow parameters that are of most interest. This approach provides a dual benefit to environmental site assessment. First, it provides a powerful set of tools for jointly inverting geophysical data; and secondly, it provides a common platform for visualizing the results. No longer will it be necessary to overlay disparate images to look for "common anomalies". Instead of comparing multiple images of electrical conductivity and seismic velocity for site information, it will be possible to will examine single images of porosity and saturation that are derived from the geophysical data.

Three-year multi-phase research approach has been employed:

- Laboratory investigations and theoretical and numerical code development
- Develop inversion code from available borehole log data to predict measured properties of cores and sediments in the core.
- Field research, collect seismic and electrical field data and use inversion code to invert field data to produce estimates of porosity and saturation in field test area

This is intended to be a significant improvement in the state-of-the-art of underground imaging, since interpretation of data collected at a contaminated site would become much less subjective. Potential users include DOE scientists and engineers responsible for characterizing contaminated sites and monitoring remediation of contaminated sites.

Potential STCG Needs Addressed

Subsurface Contaminants Focus Area		
Field Office	**STCG Number**	**STCG Title**
ID	ID-S.1.04	Real-time Field Instrumentation for Characterization and Monitoring Soils and Groundwater.
NV	NV18-9902-04S	Long-Term Monitoring of Upward and Downward Pathways in the Vadose Zone and Closure Caps
RL	RL-SS25-S	Chemical Form and Mobility of Dense, Non-Aqueous Phase Liquids in Hanford Subsurface Transport of Contaminants

EMSP Research
Lawrence Livermore National Laboratory

Project Number: 60041 **Award Year:** 1997

Project Title: Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration

Researchers: John F. Scamehorn, University of Oklahoma - Lead
Cynthia E. Palmer, Lawrence Livermore National Laboratory
Richard W. Taylor, University of Oklahoma

EM Problem Areas: Decontamination and Decommissioning (primary)
Mixed Waste
Subsurface Contamination

Science Categories/ SubCategories: Separations Chemistry / Ligand Design and Ion-exchange

URL: http://www.doe.gov /html/em52/60041.html

Synopsis

Research on colloid-enhanced ultrafiltration for the removal of radioactive cations and anions from polluted water.

> The objectives of this research are to determine the feasibility of and develop optimum conditions for the use of colloid-enhanced ultrafiltration (CEUF) methods to remove and recover radionuclides and associated toxic non-radioactive contaminants from polluted water.

The project involves use of an innovative class of separation in the study of highly toxic radioisotopes such as plutonium and the experimental capability to handle these materials. This will permit a comprehensive study of the use of colloid-enhanced ultrafiltration processes to remove and recover important radionuclide ions and associated contaminants from aqueous streams.

The colloid-enhanced ultrafiltration methods all involve the addition of water-soluble components such as polyelectrolytes and ligands to bind target ions. In many cases, a high degree of selectivity can be attained by using a ligand which specifically complexes the target ion and is then attached to a colloid such as polyelectrolyte. For example, in this work, plutonium, thorium, strontium, uranium, and lead can all be removed in a highly selective fashion with available ligands or those, which we will synthesize as part of this project. Subsequent ultrafiltration produces purified water and a homogeneous aqueous solution containing the concentrated pollutants and added colloid. Since only liquid phases are present, these techniques can be operated at steady state and are intrinsically low-energy processes. Downstream methods to separate the pollutants from the colloids and ligands concentrate the contaminants (waste minimization) for disposal and permit recycle of the colloid for reuse. These methods have been demonstrated in general in the laboratory and in field tests on actual groundwater and will be developed for the specific target ions to be studied in this investigation.

An advantage of the colloid-enhanced ultrafiltration processes to be used here is that toxic cations and anions can be simultaneously removed from the water. As an example, a cationic polyelectrolyte can be chosen to bind multivalent anions (e.g., chromate or CrO_4^{2-}) while anionic ligands which selectively bind target cations (e.g., thorium or Th4+) are themselves electrostatically bound to the polyelectrolyte. The result is removal of multivalent anionic and selective removal of cationic pollutants in a single step. After concentration of the colloids and target ions into a retentate stream by ultrafiltration, the polyelectrolyte and ligand can be regenerated by adjustment of pH and electrolyte concentration. This project would involve determination of this mixed ion removal process efficiency and optimum operating conditions for the systems of interest (e.g., selection of polyelectrolyte and ligand, highest concentration of colloid attainable during actual ultrafiltration).

The goals of this research are several:

- Optimize removal of plutonium, uranium, thorium, strontium, lead, and chromium from contaminated water using ligand-modified colloid-enhanced ultrafiltration
- Optimize recovery of colloid and ligands for reuse in the process
- Develop design parameters for scale-up of process for field demonstration

This project entails a comprehensive study of the effects of solution composition and filtration unit operating parameters on the separation efficiency and selectivity of ligand modified colloid-enhanced ultrafiltration (LM-CEUF) processes. Problem areas identified by the Office of Environmental Management addressed by this project include removal of hazardous ionic materials from groundwater, aqueous waste solutions and mixed waste. Separation and concentration of the target ions will result in a substantial reduction in the volume of material requiring long-term storage.

Potential STCG Needs Addressed

Subsurface Contaminants Focus Area		
Field Office	**STCG Number**	**STCG Title**
CH	CH-SS01-99	Remediation of Strontium-90 Contaminated Groundwater
OR	ORHY-12a	Active In Situ Dissolved Phase Treatment Systems

EMSP Research
Lawrence Livermore National Laboratory

Project Number:	60118	**Award Year:**	1997
Project Title:	Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms		
Researchers:	Mark A. Williamson, Los Alamos National Laboratory - Lead Bartley B. Ebbinghaus, Lawrence Livermore National Laboratory Alexandria Navrotsky, University of California at Davis		
EM Problem Areas:	Nuclear Materials (primary) High Level Waste		
Science Categories/ SubCategories:	Materials Science / Chemical and Structural Properties Of Storage Materials		
URL:	http://www.doe.gov /html/em52/60118.html		

Synopsis:
Research on the thermodynamic properties of various actinide-bearing waste forms.

> The objective of this research is to develop the thermodynamic data essential for developing an understanding of the chemistry and phase equilibria of the actinide bearing mineral waste form materials proposed as immobilization matrices.

The end of the Cold War raised the need for the technical community to be concerned with the disposition of excess nuclear weapon material. Excess plutonium will either be converted into mixed-oxide fuel for use in nuclear reactors or immobilized in glass or ceramic waste forms and placed in a repository. The stability and behavior of plutonium in the ceramic materials as well as the phase behavior and stability of the ceramic material in the environment is not well established. In order to provide technically sound solutions to these issues, thermodynamic data are essential in developing an understanding of the chemistry and phase equilibria of the actinide-bearing mineral waste form materials proposed as immobilization matrices. Mineral materials of interest include zircon, zirconolite, and pyrochlore. High temperature solution calorimetry is one of the most powerful techniques, sometimes the only technique, for providing the fundamental thermodynamic data needed to establish optimum material fabrication parameters, and more importantly understand and predict the behavior of the mineral materials in the environment.

The research has the following goals:

- experimentally determine the enthalpy of formation of actinide orthosilicates,
- experimentally determine the enthalpies of formation of actinide substituted zirconolite and pyrochlore, and
- develop an understanding of the bonding characteristics and stabilities of these materials.

The data generated by this fundamental thermodynamic research will contribute to the performance assessment of the actinide bearing mineral waste form materials proposed as immobilization matrices.

Potential STCG Needs Addressed

Mixed Waste Focus Area		
Field Office	**STCG Number**	**STCG Title**
NV	NV11-9801-11	Long-term Stability of Contained Waste Forms
Tanks Focus Area		
Field Office	**STCG Number**	**STCG Title**
RL	RL-WT036-S	Alternate Waste Form Development

EMSP Research
Lawrence Livermore National Laboratory

Project Number:	60319	**Award Year:**	1997
Project Title:	Thermodynamics of the Volatilization of Actinide Metals in the High-Temperature Treatment of Radioactive Wastes		
Researchers:	Martyn G. Adamson, Lawrence Livermore National Laboratory - Lead Bartley B. Ebbinghaus, Lawrence Livermore National Laboratory		
EM Problem Areas:	Nuclear Materials (primary) High Level Waste Mixed Waste Spent Nuclear Fuel		
Science Categories/ SubCategories:	Actinide Chemistry / Actinide (Heavy Element) Chemistry (primary) Inorganic Chemistry / Multiphase/Gaseous Chemistry		
URL:	http://www.doe.gov /html/em52/60319.html		

Synopsis:

Research is a detailed study of actinide elements (U, Pu and Am) under conditions relevant to the thermal destruction of actinide containing organic-based mixed and radioactive wastes.

The objective is to develop a thermodynamic understanding of actinide volatilization and partitioning/speciation in thermal processes central to the DOE/EM mixed waste program.

This research addresses several technical needs/problem areas recently identified by DOE/EM's Office of Science and Technology. In the Low-Level and Mixed Low-Level Waste problem area, emission-free destruction of organic wastes is listed as the first exemplary science need. In the TRU Waste, Plutonium Materials, and Spent Nuclear Fuel problem areas, interactions between actinides and organic residues and materials stabilization are listed as exemplary science needs. Both of these needs require high-temperature thermodynamic studies of actinides and actinide-organic interactions.

A sound basis for designing safe and effective thermal treatment systems and the ability to allay public concerns about radioactive fugitive emissions are the principal benefits of the project. The proposed work is a combination of experimental studies and thermodynamic modeling. Vapor pressure measurements will be made to determine U, Pu and possibly Am volatile species and the extent of their volatilization when UO_2/U_3O_8 , PuO_2 and AmO_2 solids are heated to temperatures of 500 to 1500°C under pyrolyzing (reducing) conditions or under oxidizing conditions (i.e. O_2 (g) + H_2O(g) mixtures) in the presence of chlorine (Cl_2 (g) or HCl(g)). Work on uranium volatilization under reducing conditions will also be performed. In parallel with the experimental effort, a complete thermodynamic database for expected actinide gaseous species will be developed from literature data, from the proposed measurements, and from data predictions using bond energy correlation and statistical thermodynamics estimation methods.

Throughout the project, the researchers will continue to estimate key thermodynamic parameters for actinide vapor species of interest and to develop the thermodynamic database of actinide elements that will be used in thermochemical prediction models.

Potential STCG Needs Addressed

Mixed Waste Focus Area		
Field Office	**STCG Number**	**STCG Title**
ID	ID-S.2.04	Physics and Chemistry of Plasma Processing

Section 4:

Current LBNL and LLNL projects sorted by primary OST Focus Area and Science Categories addressed.

Deactivation & Decommissioning Focus Area
Associated Research Projects

Actinide Chemistry

Project Number	Title	Institution	Lead Institution
60370	Rational Design of Metal Ion Sequestering Agents	Lawrence Berkeley National Laboratory	Yes

Analytical Chemistry and Instrumentation

Project Number	Title	Institution	Lead Institution
60141	Gamma Ray Imaging for Environmental Remediation	Lawrence Berkeley National Laboratory	No
65015	Three-Dimensional Positron-Sensitive Germanium Detectors	Lawrence Berkeley National Laboratory	Yes

Geochemistry

Project Number	Title	Institution	Lead Institution
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Lawrence Berkeley National Laboratory	Yes

Actinide Chemistry

Project Number	Title	Institution	Lead Institution
60319	Thermodynamics of the Volatilization of Actinide Metals in the High-Temperature Treatment of Radioactive Wastes	Lawrence Livermore National Laboratory	Yes

Analytical Chemistry and Instrumentation

Project Number	Title	Institution	Lead Institution
65015	Three-Dimensional Positron-Sensitive Germanium Detectors	Lawrence Berkeley National Laboratory	Yes

Geochemistry

Project Number	Title	Institution	Lead Institution
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Lawrence Berkeley National Laboratory	Yes

Inorganic Chemistry

Project Number	Title	Institution	Lead Institution
60296	Research Program to Investigate the Fundamental Chemistry of Technetium	Lawrence Berkeley National Laboratory	Yes

Materials Science

Project Number	Title	Institution	Lead Institution
60118	Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms	Lawrence Livermore National Laboratory	No

Actinide Chemistry

Project Number	Title	Institution	Lead Institution
65352	Developing a Fundamental Basis for the Characterization, Separation, and Disposal of Plutonium and Other Actinides in High Level Radioactive Waste: The Effect of Temperature and Electrolyte Concentrations on Actinide Speciation	Lawrence Berkeley National Laboratory	No

Analytical Chemistry and Instrumentation

Project Number	Title	Institution	Lead Institution
65015	Three-Dimensional Positron-Sensitive Germanium Detectors	Lawrence Berkeley National Laboratory	Yes

Subsurface Contaminants Focus Area
Associated Research Projects

Analytical Chemistry and Instrumentation

Project Number	Title	Institution	Lead Institution
54698	Rapid Mass Spectrometric DNA Diagnostics for Assessing Microbial Community Activity During Bioremediation	Lawrence Berkeley National Laboratory	Yes
60141	Gamma Ray Imaging for Environmental Remediation	Lawrence Berkeley National Laboratory	No
65015	Three-Dimensional Positron-Sensitive Germanium Detectors	Lawrence Berkeley National Laboratory	Yes

Geochemistry

Project Number	Title	Institution	Lead Institution
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory	Yes
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory	Yes
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory	Yes
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Lawrence Berkeley National Laboratory	Yes

Subsurface Contaminants Focus Area
Associated Research Projects

Geophysics

Project Number	Title	Institution	Lead Institution
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory	Yes
55411	Joint Inversion of Geophysical Data for Site Characterization and Restoration Monitoring	Lawrence Livermore National Laboratory	Yes
60328	High Frequency Electromagnetic Impedance Measurements for Characterization, Monitoring and Verification Efforts	Lawrence Berkeley National Laboratory	Yes

Health Science

Project Number	Title	Institution	Lead Institution
55343	Enzyme Engineering for Biodegradation of Chlorinated Organic Pollutants	Lawrence Berkeley National Laboratory	Yes

Hydrogeology

Project Number	Title	Institution	Lead Institution
54576	On the Inclusion of the Interfacial Area Between Phases in the Physical and Mathematical Description of Subsurface Multiphase Flow	Lawrence Livermore National Laboratory	No
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory	Yes
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory	Yes

Microbial Sciences

Project Number	Title	Institution	Lead Institution
55264	High Resolution Definition of Subsurface Heterogeneity for Understanding the Biodynamics of Natural Field Systems: Advancing the Ability for Scaling to Field Conditions	Lawrence Berkeley National Laboratory	Yes

Separations Chemistry

Project Number	Title	Institution	Lead Institution
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory	No

Actinide Chemistry

Project Number	Title	Institution	Lead Institution
65352	Developing a Fundamental Basis for the Characterization, Separation, and Disposal of Plutonium and Other Actinides in High Level Radioactive Waste: The Effect of Temperature and Electrolyte Concentrations on Actinide Speciation	Lawrence Berkeley National Laboratory	No
65370	Actinide-Specific Interfacial Chemistry of Monolayer Coated Mesoporous Ceramics	Lawrence Berkeley National Laboratory	No

Analytical Chemistry and Instrumentation

Project Number	Title	Institution	Lead Institution
65398	Characterization of Actinides in Simulated Alkaline Tank Waste Sludges and Leach Solutions	Lawrence Berkeley National Laboratory	No

Engineering Sciences

Project Number	Title	Institution	Lead Institution
60451	Mechanics of Bubbles in Sludges and Slurries	Lawrence Berkeley National Laboratory	No

Geochemistry

Project Number	Title	Institution	Lead Institution
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory	Yes

Geophysics

Project Number	Title	Institution	Lead Institution
60328	High Frequency Electromagnetic Impedance Measurements for Characterization, Monitoring and Verification Efforts	Lawrence Berkeley National Laboratory	Yes

Hydrogeology

Project Number	Title	Institution	Lead Institution
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory	Yes
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory	Yes

Inorganic Chemistry

Project Number	Title	Institution	Lead Institution
60296	Research Program to Investigate the Fundamental Chemistry of Technetium	Lawrence Berkeley National Laboratory	Yes

Materials Science

Project Number	Title	Institution	Lead Institution
60118	Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms	Lawrence Livermore National Laboratory	No
60362	Ion-Exchange Processes and Mechanisms in Glasses	Lawrence Berkeley National Laboratory	No

Separations Chemistry

Project Number	Title	Institution	Lead Institution
65368	Speciation, Dissolution, and Redox Reactions of Chromium Relevant to Pretreatment and Separation of High-Level Tank Wastes	Lawrence Berkeley National Laboratory	Yes

Section 5:

Site Technology Coordination Group Technology needs which the LBNL and LLNL research projects have the potential to address sorted by OST Focus Area.

Deactivation & Decommissioning Focus Area
Associated Research Needs and EMSP Projects

Actinide Chemistry

STCG Number: ID-7.2.09 Develop a Rapid Wood Radiological Contamination Monitor **Site:** ID

Fundamental Science Need: (Derived Need) Basic physics, chemical, and instrument studies are required to support efforts to develop methods and techniques for rapid radiological contamination sensing and monitoring to support decommissioning and decontamination actions.

Project Number:	Title	Institution:
60141	Gamma Ray Imaging for Environmental Remediation	Lawrence Berkeley National Laboratory

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STCG Number: RF-DD09 DECONTAMINATION OF POROUS SURFACES **Site:** RF

Fundamental Science Need: (Derived Need) Fundamental surface, materials, and chemical science studies are needed to better understand radionuclide and heavy metal adhesion to porous and non-porous surfaces for development of improved decontamination technologies.

Project Number:	Title	Institution:
60370	Rational Design of Metal Ion Sequestering Agents	Lawrence Berkeley National Laboratory

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STCG Number: RF-DD10 DECONTAMINATION OF NON-POROUS SURFACES **Site:** RF

Fundamental Science Need: (Derived Need) Fundamental surface, materials, and chemical science studies are needed to better understand radionuclide and heavy metal adhesion to porous and non-porous surfaces for development of improved decontamination technologies.

Project Number:	Title	Institution:
60370	Rational Design of Metal Ion Sequestering Agents	Lawrence Berkeley National Laboratory

Analytical Chemistry and Instrumentation

STCG Number: ID-7.2.09 Develop a Rapid Wood Radiological Contamination Monitor **Site:** ID

Fundamental Science Need: (Derived Need) Basic physics, chemical, and instrument studies are required to support efforts to develop methods and techniques for rapid radiological contamination sensing and monitoring to support decommissioning and decontamination actions.

Project Number:	Title	Institution:
60141	Gamma Ray Imaging for Environmental Remediation	Lawrence Berkeley National Laboratory

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STCG Number: ID-S.2.05 Understanding the Physics and Chemistry of Concrete Decontamination **Site:** ID

Fundamental Science Need: (STCG Science Need) Fundamental studies are needed on physical/chemical binding of radionuclides to bare and weathered concrete and painted concrete surfaces. Mesoscale modeling and experiments are needed to characterize flow and percolation of fluids through porous and fractured concrete surfaces. The influence of chemical, mechanical, and biological processes on the physical properties and fracture of concrete require characterization. These data will lead to the development of more efficient chemical and biological processes for decontamination.

Project Number:	Title	Institution:
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Lawrence Berkeley National Laboratory

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STCG Number: RL-DD023-S Cesuim Source Identification **Site:** RL

Fundamental Science Need: (STCG Science Need) An understanding of processes to locate a leak from the cesium chloride capsules is needed in order to develop a means of identifying leaking capsules quickly. Since cesium is highly soluble, some other material may act as a leaker identifying agent.

Project Number:	Title	Institution:
60141	Gamma Ray Imaging for Environmental Remediation	Lawrence Berkeley National Laboratory
65015	Three-Dimensional Positron-Sensitive Germanium Detectors	Lawrence Berkeley National Laboratory

Engineering Sciences

STCG Number: ID-S.2.05 Understanding the Physics and Chemistry of Concrete Decontamination **Site:** ID

Fundamental Science Need: (STCG Science Need)
Fundamental studies are needed on physical/chemical binding of radionuclides to bare and weathered concrete and painted concrete surfaces. Mesoscale modeling and experiments are needed to characterize flow and percolation of fluids through porous and fractured concrete surfaces. The influence of chemical, mechanical, and biological processes on the physical properties and fracture of concrete require characterization. These data will lead to the development of more efficient chemical and biological processes for decontamination.

Project Number:	Title	Institution:
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Lawrence Berkeley National Laboratory

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STCG Number: RF-DD09 DECONTAMINATION OF POROUS SURFACES **Site:** RF

Fundamental Science Need: (Derived Need)
Fundamental surface, materials, and chemical science studies are needed to better understand radionuclide and heavy metal adhesion to porous and non-porous surfaces for development of improved decontamination technologies.

Project Number:	Title	Institution:
60370	Rational Design of Metal Ion Sequestering Agents	Lawrence Berkeley National Laboratory

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STCG Number: RF-DD10 DECONTAMINATION OF NON-POROUS SURFACES **Site:** RF

Fundamental Science Need: (Derived Need)
Fundamental surface, materials, and chemical science studies are needed to better understand radionuclide and heavy metal adhesion to porous and non-porous surfaces for development of improved decontamination technologies.

Project Number:	Title	Institution:
60370	Rational Design of Metal Ion Sequestering Agents	Lawrence Berkeley National Laboratory

Geochemistry

STCG Number: RF-DD09 DECONTAMINATION OF POROUS SURFACES **Site:** RF

Fundamental Science Need: (Derived Need) Fundamental surface, materials, and chemical science studies are needed to better understand radionuclide and heavy metal adhesion to porous and non-porous surfaces for development of improved decontamination technologies.

Project Number:	Title	Institution:
60370	Rational Design of Metal Ion Sequestering Agents	Lawrence Berkeley National Laboratory

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STCG Number: RL-DD026-S Contaminant Binding Science Need **Site:** RL

Fundamental Science Need: (STCG Science Need) An understanding is needed of contamination chemistry and their binding mechanism to contaminated surfaces, decontaminants and fixatives to allow for optimal methods to be developed.

Project Number:	Title	Institution:
60370	Rational Design of Metal Ion Sequestering Agents	Lawrence Berkeley National Laboratory

Inorganic Chemistry

STCG Number: ID-7.2.09 Develop a Rapid Wood Radiological Contamination Monitor **Site:** ID

Fundamental Science Need: (Derived Need) Basic physics, chemical, and instrument studies are required to support efforts to develop methods and techniques for rapid radiological contamination sensing and monitoring to support decommissioning and decontamination actions.

Project Number:	Title	Institution:
60141	Gamma Ray Imaging for Environmental Remediation	Lawrence Berkeley National Laboratory

STCG Number: RF-DD09 DECONTAMINATION OF POROUS SURFACES **Site:** RF

Fundamental Science Need: (Derived Need) Fundamental surface, materials, and chemical science studies are needed to better understand radionuclide and heavy metal adhesion to porous and non-porous surfaces for development of improved decontamination technologies.

Project Number:	Title	Institution:
60370	Rational Design of Metal Ion Sequestering Agents	Lawrence Berkeley National Laboratory

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STCG Number: RF-DD10 DECONTAMINATION OF NON-POROUS SURFACES **Site:** RF

Fundamental Science Need: (Derived Need) Fundamental surface, materials, and chemical science studies are needed to better understand radionuclide and heavy metal adhesion to porous and non-porous surfaces for development of improved decontamination technologies.

Project Number:	Title	Institution:
60370	Rational Design of Metal Ion Sequestering Agents	Lawrence Berkeley National Laboratory

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STCG Number: RL-DD026-S Contaminant Binding Science Need **Site:** RL

Fundamental Science Need: (STCG Science Need) An understanding is needed of contamination chemistry and their binding mechanism to contaminated surfaces, decontaminants and fixatives to allow for optimal methods to be developed.

Project Number:	Title	Institution:
60370	Rational Design of Metal Ion Sequestering Agents	Lawrence Berkeley National Laboratory

Materials Science

STCG Number: ID-S.2.05 — Understanding the Physics and Chemistry of Concrete Decontamination — **Site:** ID

Fundamental Science Need:
(STCG Science Need)

Fundamental studies are needed on physical/chemical binding of radionuclides to bare and weathered concrete and painted concrete surfaces. Mesoscale modeling and experiments are needed to characterize flow and percolation of fluids through porous and fractured concrete surfaces. The influence of chemical, mechanical, and biological processes on the physical properties and fracture of concrete require characterization. These data will lead to the development of more efficient chemical and biological processes for decontamination.

Project Number:	Title	Institution:
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Lawrence Berkeley National Laboratory

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STCG Number: RF-DD09 — DECONTAMINATION OF POROUS SURFACES — **Site:** RF

Fundamental Science Need:
(Derived Need)

Fundamental surface, materials, and chemical science studies are needed to better understand radionuclide and heavy metal adhesion to porous and non-porous surfaces for development of improved decontamination technologies.

Project Number:	Title	Institution:
60370	Rational Design of Metal Ion Sequestering Agents	Lawrence Berkeley National Laboratory

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STCG Number: RF-DD10 — DECONTAMINATION OF NON-POROUS SURFACES — **Site:** RF

Fundamental Science Need:
(Derived Need)

Fundamental surface, materials, and chemical science studies are needed to better understand radionuclide and heavy metal adhesion to porous and non-porous surfaces for development of improved decontamination technologies.

Project Number:	Title	Institution:
60370	Rational Design of Metal Ion Sequestering Agents	Lawrence Berkeley National Laboratory

STCG Number:	RL-DD026-S	Contaminant Binding Science Need	**Site:**	RL
Fundamental Science Need: (STCG Science Need)		An understanding is needed of contamination chemistry and their binding mechanism to contaminated surfaces, decontaminants and fixatives to allow for optimal methods to be developed.		

Project Number:	**Title**	**Institution:**
60370	Rational Design of Metal Ion Sequestering Agents	Lawrence Berkeley National Laboratory

Actinide Chemistry

STCG Number: AL-09-01-24-MW-S — Radioassay of Remote-Handled Transuranic (RH-TRU) Waste Containers to Meet WIPP Data Quality — **Site:** AL

Fundamental Science Need: (STCG Science Need)

Two difficult science problems associated with RH-TRU waste containers that are to be shipped to WIPP are (1) determining that the 239Pu Fissile Gram Equivalent content is less that the 325 gram limit, and (2) determining that the thermal power is less than 50 watts for combustible waste containers, and less than 300 watts for noncombustible waste containers. In RH-TRU waste, the plutonium radiation signal is small compared to the very large background of radiation from fission products. New radioassay techniques need to be developed that can determine a small fission neutron or gamma-ray signal in the presence of a high gamma-ray background. Specific approaches including time discrimination of correlated fission gammas or neutrons, energy discrimination, high-Z shielding, fiber neutron capture detectors, and fast neutron telescopes need further investigation. Design of experimental setups, benchmark measurements of CH and RH-TRU waste, and new data analysis algorithms are all needed. Comparison and peer review of several different approaches is also needed to see which are best for the various categories of RH-TRU waste in the DOE complex. The thermal power output of RH-TRU waste can be determined by calculation if the radioisotope inventory is known, or by direct heat measurement using radiometric calorimetry. The latter approach is a well-established technique for small nuclear material containers, but requires additional research to develop a calorimeter large enough to measure RH-TRU waste drums. Depending on the performance that can be achieved, the calorimetry measurement might provide a verification of the calculated thermal power, or a direct measurement. Measurements of the RH-TRU fissile content or thermal power are critically needed so that this waste category, which is very difficult and costly to handle, can be removed from storage at several DOE sites and transported safely to WIPP.

Project Number:	Title	Institution:
65015	Three-Dimensional Positron-Sensitive Germanium Detectors	Lawrence Berkeley National Laboratory

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STCG Number: AL-09-01-25-MW-S — Radioassay of Very Large Containers of Low-Level Contact-Handled Transuranic (CH-TRU) Waste to Meet WIPP Data Quality Assurance Objectives — **Site:** AL

Fundamental Science Need: (STCG Science Need)

Two science problems associated with very large CH-TRU waste containers like B-25 boxes and Sea-Land containers that are to be shipped to WIPP or buried as non-radioactive waste are (1) determining that the 239Pu Fissile Gram Equivalent content is less that the325 gram limit, and (2) determining that the TRU content is less than 100 nanocuries per gram or 10 nanocuries per gram. For very large containers, even neutrons may not penetrate to the surface, depending on the matrix materials that are present. To determine the 239Pu Fissile Gram Equivalent content accurately, new radioassay correction algorithms based on neutron emission and transmission tomography, new gamma-ray transmission corrections, and additional matrix identification techniques need to be developed. The goal is to improve cleanup cost and throughput by increase the amount of plutonium that can be shipped within the WIPP uncertainty limits. For screening of very large containers at the 10 or 100 nanocurie per gram limit, new background reduction techniques need to be developed to deal with external backgrounds and internal backgrounds due to spallation neutrons from cosmic ray sources. The goal is to improve cleanup cost and throughput by reducing the number of containers that need to be shipped to WIPP because of limitations in the screening techniques.

Project Number:	Title	Institution:
65015	Three-Dimensional Positron-Sensitive Germanium Detectors	Lawrence Berkeley National Laboratory

Analytical Chemistry and Instrumentation

STCG Number: AL-09-01-24-MW-S — Radioassay of Remote-Handled Transuranic (RH-TRU) Waste Containers to Meet WIPP Data Quality — **Site:** AL

Fundamental Science Need: (STCG Science Need)

Two difficult science problems associated with RH-TRU waste containers that are to be shipped to WIPP are (1) determining that the239Pu Fissile Gram Equivalent content is less that the 325 gram limit, and (2) determining that the thermal power is less than 50 watts for combustible waste containers, and less than 300 watts for noncombustible waste containers. In RH-TRU waste, the plutonium radiation signal is small compared to the very large background of radiation from fission products. New radioassay techniques need to be developed that can determine a small fission neutron or gamma-ray signal in the presence of a high gamma-ray background. Specific approaches including time discrimination of correlated fission gammas or neutrons, energy discrimination, high-Z shielding, fiber neutron capture detectors, and fast neutron telescopes need further investigation. Design of experimental setups, benchmark measurements of CH and RH-TRU waste, and new data analysis algorithms are all needed. Comparison and peer review of several different approaches is also needed to see which are best for the various categories of RH-TRU waste in the DOE complex. The thermal power output of RH-TRU waste can be determined by calculation if the radioisotope inventory is known, or by direct heat measurement using radiometric calorimetry. The latter approach is a well-established technique for small nuclear material containers, but requires additional research to develop a calorimeter large enough to measure RH-TRU waste drums. Depending on the performance that can be achieved, the calorimetry measurement might provide a verification of the calculated thermal power, or a direct measurement. Measurements of the RH-TRU fissile content or thermal power are critically needed so that this waste category, which is very difficult and costly to handle, can be removed from storage at several DOE sites and transported safely to WIPP.

Project Number:	Title	Institution:
65015	Three-Dimensional Positron-Sensitive Germanium Detectors	Lawrence Berkeley National Laboratory

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STCG Number: AL-09-01-25-MW-S — Radioassay of Very Large Containers of Low-Level Contact-Handled Transuranic (CH-TRU) Waste to Meet WIPP Data Quality Assurance Objectives — **Site:** AL

Fundamental Science Need: (STCG Science Need)

Two science problems associated with very large CH-TRU waste containers like B-25 boxes and Sea-Land containers that are to be shipped to WIPP or buried as non-radioactive waste are (1) determining that the 239Pu Fissile Gram Equivalent content is less that the325 gram limit, and (2) determining that the TRU content is less than 100 nanocuries per gram or 10 nanocuries per gram. For very large containers, even neutrons may not penetrate to the surface, depending on the matrix materials that are present. To determine the 239Pu Fissile Gram Equivalent content accurately, new radioassay correction algorithms based on neutron emission and transmission tomography, new gamma-ray transmission corrections, and additional matrix identification techniques need to be developed. The goal is to improve cleanup cost and throughput by increase the amount of plutonium that can be shipped within the WIPP uncertainty limits. For screening of very large containers at the 10 or 100 nanocurie per gram limit, new background reduction techniques need to be developed to deal with external backgrounds and internal backgrounds due to spallation neutrons from cosmic ray sources. The goal is to improve cleanup cost and throughput by reducing the number of containers that need to be shipped to WIPP because of limitations in the screening techniques.

Project Number:	Title	Institution:

65015	Three-Dimensional Positron-Sensitive Germanium Detectors	Lawrence Berkeley National Laboratory

STCG Number: ID-S.1.05 Nondestructive Assay (NDA) Capability for Remote-Handled Transuranic Waste **Site:** ID

Fundamental Science Need: (STCG Science Need)

There is a need for nondestructive Assay (NDA) ability to characterize Remote-Handled Transuranic (RH-TRU) for shipment of waste for direct or offsite disposal. The method or technique used must have the capacity to assay materials having significant radiation fields (typically ranging from 5 to 20 R). The assay method is needed so that determination of the isotopic composition, actinide concentrations, and total alpha activity of the material can be quantitated. Fundamental studies associated with methods development, gamma and neutron based detection approaches, development of analysis algorithms, and improved sources of neutrons are needed to identify actinide elements, reduce spectral complications produced by uranium reactor fuel and cladding fission products, reduce measurement uncertainty, and understand waste matrix gamma and neutron transmission.

Project Number:	Title	Institution:
65015	Three-Dimensional Positron-Sensitive Germanium Detectors	Lawrence Berkeley National Laboratory

STCG Number: ID-S.2.02 Nondestructive Assay (NDA) for Resource Conservation and Recovery Act Metal and Chlorine in Incinerator **Site:** ID

Fundamental Science Need: (STCG Science Need)

There is a need for nondestructive assay (NDA) ability to characterize Resource Conservation and Recovery Act (RCRA) metals and organic chlorine content in each package of heterogeneous, non-uniformly contaminated incinerator feed. Airborne emissions of antimony, barium, lead, mercury, nickel, selenium, silver, thallium, arsenic, beryllium, cadmium, chromium, and hydrochloric acid are controlled by adjusting the incinerator feed rates of these constituents in the waste. Fundamental studies leading to development of improved (sensitivity) gamma detectors, refinement of gamma analysis algorithms, and higher intensity neutron sources are needed to reduce minimum detectable concentration limits associated with gamma based NDA approaches.

Project Number:	Title	Institution:
65015	Three-Dimensional Positron-Sensitive Germanium Detectors	Lawrence Berkeley National Laboratory

STCG Number: ID-S.2.04 Physics and Chemistry of Plasma Processing **Site:** ID

Fundamental Science Need: (STCG Science Need)

The development of both theoretical and experimental tools that will allow control (through better design and operation) of the reactions that occur in plasma processing is needed to enable plasma processing to treat hazardous waste effectively and consistently, and, when possible, produce useful non-hazardous byproducts from the waste thereby minimizing the creation of secondary waste streams.

Project Number:	Title	Institution:
60319	Thermodynamics of the Volatilization of Actinide Metals in the High-Temperature Treatment of Radioactive	Lawrence Livermore National Laboratory

STCG Number: None — NDA for TRU in drums, boxes, and mics. Debris — **Site:** ID

Fundamental Science Need: (STCG Science Need)
Detection and isotopic differentiation of low levels of transuranic elements in a wide variety of wastes packaged in assorted containers is essential to reducing the costs of waste disposition. Basic research in new detection concepts, or definitive work in establishing the absolute limits for what can be measured would support sorting, characterizing, and treatment of alpha contaminated wastes.

Project Number:	Title	Institution:
65015	Three-Dimensional Positron-Sensitive Germanium Detectors	Lawrence Berkeley National Laboratory

Fundamental Science Need: (STCG Science Need)
Detection and differentiation of environmentally regulated elements in a wide variety of wastes packaged in assorted containers is essential to reducing the costs of waste disposition. Basic research in new detection concepts, or definitive work in establishing the absolute limits for what can be measured would support sorting, characterizing, and treatment of mixed wastes. Similar detection capability for chlorine would support more efficient use of current incineration capacity.

Project Number:	Title	Institution:
65015	Three-Dimensional Positron-Sensitive Germanium Detectors	Lawrence Berkeley National Laboratory

Engineering Sciences

STCG Number: ID-S.2.04 — Physics and Chemistry of Plasma Processing — **Site:** ID

Fundamental Science Need: (STCG Science Need)
The development of both theoretical and experimental tools that will allow control (through better design and operation) of the reactions that occur in plasma processing is needed to enable plasma processing to treat hazardous waste effectively and consistently, and, when possible, produce useful non-hazardous byproducts from the waste thereby minimizing the creation of secondary waste streams

Project Number:	Title	Institution:
60319	Thermodynamics of the Volatilization of Actinide Metals in the High-Temperature Treatment of Radioactive	Lawrence Livermore National Laboratory

STCG Number: NV11-9801-11 Long-term Stability of Contained Waste Forms **Site:** NV

Fundamental Science Need: (Derived Need) Fundamental geoscience, geochemistry and materials science studies are desired to understand the long-term stability of contained waste forms to support disposal facility/site performance assessments.

Project Number:	Title	Institution:
60118	Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms	Lawrence Livermore National Laboratory

Inorganic Chemistry

STCG Number: None Metal ion binding in sludges, sediments and soils **Site:** ID

Fundamental Science Need: (STCG Science Need) Greater understanding of how radioactive or environmentally regulated ions are bounding fine materials could be used to design flowsheets for decontamination, or treatment of fix materials permanently to reduce the risk in disposal.

Project Number:	Title	Institution:
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Lawrence Berkeley National Laboratory

STCG Number: SR99-2049-S Technetium Chemistry Under Waste Removal Conditions **Site:** SR

Fundamental Science Need: (STCG Science Need) A better understanding of the chemistry of technetium and other significant waste contaminants is needed to improve waste removal in preparation for tank closure.

Project Number:	Title	Institution:
60296	Research Program to Investigate the Fundamental Chemistry of Technetium	Lawrence Berkeley National Laboratory

Materials Science

STCG Number: ID-S.2.04 — Physics and Chemistry of Plasma Processing — **Site:** ID

Fundamental Science Need: (STCG Science Need)
The development of both theoretical and experimental tools that will allow control (through better design and operation) of the reactions that occur in plasma processing is needed to enable plasma processing to treat hazardous waste effectively and consistently, and, when possible, produce useful non-hazardous byproducts from the waste thereby minimizing the creation of secondary waste streams.

Project Number:	Title	Institution:
60319	Thermodynamics of the Volatilization of Actinide Metals in the High-Temperature Treatment of Radioactive	Lawrence Livermore National Laboratory

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STCG Number: None — Metal ion binding in sludges, sediments and soils — **Site:** ID

Fundamental Science Need: (STCG Science Need)
Greater understanding of how radioactive or environmentally regulated ions are bounding fine materials could be used to design flowsheets for decontamination, or treatment of fix materials permanently to reduce the risk in disposal.

Project Number:	Title	Institution:
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Lawrence Berkeley National Laboratory

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STCG Number: NV11-9801-11 — Long-term Stability of Contained Waste Forms — **Site:** NV

Fundamental Science Need: (Derived Need)
Fundamental geoscience, geochemistry and materials science studies are desired to understand the long-term stability of contained waste forms to support disposal facility/site performance assessments.

Project Number:	Title	Institution:
60118	Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms	Lawrence Livermore National Laboratory

Separations Chemistry

STCG Number: SR99-2049-S Technetium Chemistry Under Waste Removal Conditions **Site:** SR

Fundamental Science Need: (STCG Science Need) A better understanding of the chemistry of technetium and other significant waste contaminants is needed to improve waste removal in preparation for tank closure.

Project Number:	Title	Institution:
60296	Research Program to Investigate the Fundamental Chemistry of Technetium	Lawrence Berkeley National Laboratory

Actinide Chemistry

STCG Number: AL-09-01-23-Pu- S — Selective Aqueous Non-invasive Extractions of Low and Medium Fired PuO2 from High Level Wastes, Residues, and Concentrates — **Site:** AL

Fundamental Science Need: (STCG Science Need)

There are many TRU wastes that contain high levels of Pu that are beyond the criticality or gas generation limits for shipment to the WIPP or some storage location. A process and methodology is needed to have the option to selectively extract the PuO2 from the residues, ashes, or waste matrixes without significantly dissolving the matrix. This need includes not developing a significant secondary waste stream. Fundamental Scientific Understanding Needed: The fundamental science that is needed is to empirically determine the compounds that can effectively dissolve medium-fired PuO2 within 10 min without dissolving the matrix. The optimal temperature and acid conditions for selective and rapid dissolution must be established. Technology solution that will be implemented when Scientific Understanding above is achieved: A process and methodology that allows selective extraction and concentration of Pu with a rapid chemical wash and allows concentration of the resultant Pu salt so that residual waste can be disposed of as a low level waste without criticality or gas generation concerns. Resultant reduction in cost, schedule, ES&H, and/or risk: This technology will provide a new methodology that can be used for D&D operations and waste preparations for disposal at the WIPP. This will reduce the source term in the waste and the environment and will significantly lower the cost of disposal.

Project Number:	Title	Institution:
65352	Developing a Fundamental Basis for the Characterization, Separation, and Disposal of Plutonium and Other Actinides in High Level Radioactive Waste: The Effect of Temperature and Electrolyte Concentrations on Actinide Speciation	Lawrence Berkeley National Laboratory

Analytical Chemistry and Instrumentation

STCG Number: RF-WM04 — IMPROVED SENSITIVITY FOR PLUTONIUM ASSAY INSTRUMENTATION — **Site:** RF

Fundamental Science Need: (Derived Need)

Basic physics and instrument science is requested to support improved nondestructive assay for low and high concentration of plutonium in the presence of uranium, americium, and neptunium.

Project Number:	Title	Institution:
65015	Three-Dimensional Positron-Sensitive Germanium Detectors	Lawrence Berkeley National Laboratory

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STCG Number: RF-WM04-98 — IMPROVED SENSITIVITY FOR PLUTONIUM NON-DESTRUCTIVE ASSAY (NDA) INSTRUMENTATION — **Site:** RF

Fundamental Science Need: (Derived Need)

Basic physics and instrument science is requested to support improved nondestructive assay for low and high concentration of plutonium in the presence of uranium, americium, and neptunium.

Project Number:	Title	Institution:

65015	Three-Dimensional Positron-Sensitive Germanium Detectors	Lawrence Berkeley National Laboratory

Separations Chemistry

STCG Number:	AL-09-01-23-Pu- S	Selective Aqueous Non-invasive Extractions of Low and Medium Fired PuO2 from High Level Wastes, Residues, and Concentrates	**Site:**	AL

Fundamental Science Need:
(STCG Science Need)

There are many TRU wastes that contain high levels of Pu that are beyond the criticality or gas generation limits for shipment to the WIPP or some storage location. A process and methodology is needed to have the option to selectively extract the PuO2 from the residues, ashes, or waste matrixes without significantly dissolving the matrix. This need includes not developing a significant secondary waste stream. Fundamental Scientific Understanding Needed: The fundamental science that is needed is to empirically determine the compounds that can effectively dissolve medium-fired PuO2 within 10 min without dissolving the matrix. The optimal temperature and acid conditions for selective and rapid dissolution must be established. Technology solution that will be implemented when Scientific Understanding above is achieved: A process and methodology that allows selective extraction and concentration of Pu with a rapid chemical wash and allows concentration of the resultant Pu salt so that residual waste can be disposed of as a low level waste without criticality or gas generation concerns. Resultant reduction in cost, schedule, ES&H, and/or risk: This technology will provide a new methodology that can be used for D&D operations and waste preparations for disposal at the WIPP. This will reduce the source term in the waste and the environment and will significantly lower the cost of disposal.

Project Number:	Title	Institution:
65352	Developing a Fundamental Basis for the Characterization, Separation, and Disposal of Plutonium and Other Actinides in High Level Radioactive Waste: The Effect of Temperature and Electrolyte Concentrations on Actinide Speciation	Lawrence Berkeley National Laboratory

Actinide Chemistry

STCG Number: ID-S.1.04 — Real-time Field Instrumentation for Characterization and Monitoring Soils and Groundwater. **Site:** ID

Fundamental Science Need: (STCG Science Need)

There are a number of scientific issues associated with the need for field instrumentation to perform real-time characterization and monitoring tasks. In order to gain the speed necessary to produce near real time measurements it is generally necessary to enhance sensitivity. For optical devices this implies the development of new detector materials or detection devices or faster means of sample concentration. For other types of sensors as well there is the need to provide fast sample concentration and preconditioning. Basic research in separations technologies for water/organic contaminant systems is needed. Speciation information for RCRA metals and radionuclides in varying geologic environments is necessary to understand what mobilization and separation technologies can be applied or need to be developed. The radionuclides of concern and the levels to which they need to be detected are (within 1 pCi/g) Cs-137 at16 pCi/g, Sr-90 at 60 pCi/g, Co-60 at 1.8E+5 pCi/g, and Eu-152 at 140 pCi/g.

Project Number:	Title	Institution:
55411	Joint Inversion of Geophysical Data for Site Characterization and Restoration Monitoring	Lawrence Livermore National Laboratory
60328	High Frequency Electromagnetic Impedance Measurements for Characterization, Monitoring and Verification	Lawrence Berkeley National Laboratory
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

Analytical Chemistry and Instrumentation

STCG Number: AL-09-01-27-SC-S — Long-term Monitoring Sensor Technology **Site:** AL

Fundamental Science Need: (STCG Science Need)

Monitoring of environmental legacy sites will be required for a 30 to 100 year period after completion of initial characterization and remediation actions. A science foundation is needed that can support the development of new and innovative sensor systems that can significantly decrease the cost as well as improve performance of this long-term environmental surveillance and monitoring requirement. Background: Commitments to continued site monitoring are typically made to regulators during negotiations on the completion of remediation activities and legacy site closure. These commitments to monitoring extend for periods of time ranging from 30 to 100 years. The intent of long-term surveillance and monitoring is to verify that remediation efforts have met site goals and that no unexpected contaminant releases have occurred. For some sites, the cost of long-term monitoring over decades can equal or exceed the original remediation cost. Science Gaps: The scientific basis to create and gain acceptance of innovative sensors needs to be significantly enhanced. Specifically, sensors to measure in situ contaminants (radionuclides, organics, and metals), geophysical, and geo-hydraulic properties and to provide real-time information are needed.

Project Number:	Title	Institution:
60141	Gamma Ray Imaging for Environmental Remediation	Lawrence Berkeley National Laboratory

STCG Number: ID-6.1.01 In-Situ Debris Characterization for Partial Retrieval **Site:** ID

Fundamental Science Need: (Derived Need) Basic geophysical, physics, chemical, and instrumental studies are needed to develop improved in situ analytical determination of hazardous species associated with buried debris waste forms.

Project Number:	Title	Institution:
65015	Three-Dimensional Positron-Sensitive Germanium Detectors	Lawrence Berkeley National Laboratory
60141	Gamma Ray Imaging for Environmental Remediation	Lawrence Berkeley National Laboratory

STCG Number: ID-S.1.04 Real-time Field Instrumentation for Characterization and Monitoring Soils and Groundwater. **Site:** ID

Fundamental Science Need: (STCG Science Need) There are a number of scientific issues associated with the need for field instrumentation to perform real-time characterization and monitoring tasks. In order to gain the speed necessary to produce near real time measurements it is generally necessary to enhance sensitivity. For optical devices this implies the development of new detector materials or detection devices or faster means of sample concentration. For other types of sensors as well there is the need to provide fast sample concentration and preconditioning. Basic research in separations technologies for water/organic contaminant systems is needed. Speciation information for RCRA metals and radionuclides in varying geologic environments is necessary to understand what mobilization and separation technologies can be applied or need to be developed. The radionuclides of concern and the levels to which they need to be detected are (within 1 pCi/g) Cs-137 at16 pCi/g, Sr-90 at 60 pCi/g, Co-60 at 1.8E+5 pCi/g, and Eu-152 at 140 pCi/g.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55411	Joint Inversion of Geophysical Data for Site Characterization and Restoration Monitoring	Lawrence Livermore National Laboratory
60328	High Frequency Electromagnetic Impedance Measurements for Characterization, Monitoring and Verification	Lawrence Berkeley National Laboratory
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory

STCG Number: ID-S.2.01 — Definition of ´Biologically Active Zones´ in Fractured Rock Environments — **Site:** ID

Fundamental Science Need: (STCG Science Need)
Fundamental understanding of biogeochemical reactions (including rates and extents) with contaminants in the subsurface as they are related to specific conditions (e.g. fractures, rubble zones, interbeds) such that biologically active zones can be predicted and evaluated more effectively.

Project Number:	Title	Institution:
54698	Rapid Mass Spectrometric DNA Diagnostics for Assessing Microbial Community Activity During Bioremediation	Lawrence Berkeley National Laboratory
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory

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STCG Number: NV18-9902-04S — Long-Term Monitoring of Upward and Downward Pathways in the Vadose Zone and Closure Caps — **Site:** NV

Fundamental Science Need: (STCG Science Need)
Monitoring of low-level waste disposal and mixed waste sites is a requirement for meeting DOE Order 5820.2A and RCRA regulations, respectively. Efficient vadose zone monitoring systems capable of responding to regulatory requirements need to be designed, demonstrated, and deployed at the radioactive waste management sites. These systems need to provide early warning of the potential for or a measurable increase in the rates of transport of waste radionuclides along transport pathways. Additionally, they need to provide data to reduce uncertainty and test conceptual models and assumptions and parameters in performance assessment studies. Optimization of instrument packages, deployment geometry, and detection capability for the NTS setting is needed. Aproposal to deploy a monolayer-ET cover on an Area 3 waste cell is planned under the ASTD program.

Project Number:	Title	Institution:
55411	Joint Inversion of Geophysical Data for Site Characterization and Restoration Monitoring	Lawrence Livermore National Laboratory
60328	High Frequency Electromagnetic Impedance Measurements for Characterization, Monitoring and Verification	Lawrence Berkeley National Laboratory
55264	High Resolution Definition of Subsurface Heterogeneity for Understanding the Biodynamics of Natural Field Systems: Advancing the Ability for Scaling to Field Conditions	Lawrence Berkeley National Laboratory
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

STCG Number: OK99-20 Innovative Technology to Investigate Geology and Groundwater Flow Characteristics in Fractured Rock **Site:** OK

Fundamental Science Need: (Derived Need) Fundamental geoscience, hydrology, and fluid flow studies are desired to understand groundwater flow through fractured rock.

Project Number:	Title	Institution:
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

Bioremediation

STCG Number: AL-07-04-01-SC Non-Itrusive Removal of Polychlorinated Biphenols (PCBs) from Soil Both Above and Below the Water Table Underneath Buildings **Site:** AL

Fundamental Science Need: (Derived Need) Chemical and microbial science studies are needed to support non-intrusive removal of polychlorinated biphenol from soils located underneath buildings.

Project Number:	Title	Institution:
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Lawrence Berkeley National Laboratory

STCG Number: AL-07-06-04-SC — In Situ Remediation Of HE, Solvents, VOCs, SVOCs, Heavy Metals, And Landfill Materials — **Site:** AL

Fundamental Science Need: (Derived Need)
Fundamental study of reacting flows in heterogeneous porous media, heat transfer, chemistry, microbial and engineering sciences are needed to support efforts to develop technologies for in situ remediation of high explosives, solvents, volatile organic compounds, semi-volatile organic compounds, heavy metals, and landfill materials.

Project Number:	Title	Institution:
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Lawrence Berkeley National Laboratory
55343	Enzyme Engineering for Biodegradation of Chlorinated Organic Pollutants	Lawrence Berkeley National Laboratory

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STCG Number: ID-6.1.04 — In-situ Treatment of VOC Contaminated Groundwater in Deep Fractured Rock — **Site:** ID

Fundamental Science Need: (Derived Need)
Basic microbial, chemical, and geochemical studies are desired to support development of an in situ method for treatment of volatile organic contaminants in groundwater located in deep fracture rock environments.

Project Number:	Title	Institution:
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory

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STCG Number: ORHY-12a — Active In Situ Dissolved Phase Treatment Systems — **Site:** OR

Fundamental Science Need: (Derived Need)
Fundamental study of reacting flows in heterogeneous porous media, heat transfer, chemistry, microbial and engineering sciences are needed to support efforts to develop technologies for in situ remediation of high explosives, solvents, volatile organic compounds, semi-volatile organic compounds, heavy metals, and landfill materials.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory

60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory

Fundamental Science Need: (Derived Need)

Basic microbial, chemical, and geochemical studies are desired to support development of an in situ method for treatment of volatile organic contaminants in groundwater located in deep fracture rock environments.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory

Fundamental Science Need: (Derived Need)

Basic biological and biochemical studies are needed to understand biological metabolism (single species and consortia) of halogenated organic compounds and metal/radionuclide organic complex in subsurface hydrogeological environments.

Project Number:	Title	Institution:
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory

55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory

Fundamental Science Need: (Derived Need)

Basic chemistry, geochemical, and fluid flow studies are needed to understand movement of contaminant (Tc, Sc, U, Cs, and Sr) through zones of low moisture and to understand the movement of water as liquid and vapor phases and retention of water on particle surfaces that improve dose calculations.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory

Engineering Sciences

STCG Number: AL-09-01-03-SC-S — Succession and Long-Term Performance of Landfill Covers — **Site:** AL

Fundamental Science Need: (STCG Science Need)

The vast majority of contamination at DOE sites will be left in situ and stabilized with an engineered landfill cover. Although many studies have evaluated the initial performance of landfill cover designs over a few years, lacking are studies that determine the long-term integrity of covers and how they will change with plant succession and associated processes. Field studies of succession and use of natural analogs for determining the long-term performance of landfill covers are needed, as called for at the December 1998 special section on Landfill Covers at the American Geophysical Union meeting. Further, modeling that integrates hydrology of covers, succession, and risk is totally lacking and needed to address this problem.

Project Number:	Title	Institution:
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory

54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

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STCG Number: ID-6.1.01 In-Situ Debris Characterization for Partial Retrieval **Site:** ID

Fundamental Science Need: (Derived Need) Basic geophysical, physics, chemical, and instrumental studies are needed to develop improved in situ analytical determination of hazardous species associated with buried debris waste forms.

Project Number:	Title	Institution:
65015	Three-Dimensional Positron-Sensitive Germanium Detectors	Lawrence Berkeley National Laboratory
60141	Gamma Ray Imaging for Environmental Remediation	Lawrence Berkeley National Laboratory

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STCG Number: ORHY-01a Dense Non-Aqueous Phase Liquid (DNAPL) Source Characterization, Containment, and Treatment **Site:** OR

Fundamental Science Need: (Derived Need) Basic microbial, chemical, and engineering science studies associated with characterization, and remediation of carbon tetrachloride as a dense nonaqueous phase liquid in the subsurface is needed to support closure of the Rocky Flats plant.

Project Number:	Title	Institution:
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory

Fundamental Science Need: (Derived Need) Basic geochemical and chemical investigations are needed to understand changes to steady state chemistry of carbon tetrachloride degradation due to manipulation of subsurface conditions either by emplacement of containment materials or by addition of chemicals that alter oxidation/reduction potential of the aquifer.

Project Number:	Title	Institution:
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory

55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory

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STCG Number: ORHY-12a Active In Situ Dissolved Phase Treatment Systems **Site:** OR

Fundamental Science Need:
(Derived Need)

Fundamental study of reacting flows in heterogeneous porous media, heat transfer, chemistry, microbial and engineering sciences are needed to support efforts to develop technologies for in situ remediation of high explosives, solvents, volatile organic compounds, semi-volatile organic compounds, heavy metals, and landfill materials.

Project Number:	Title	Institution:
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

Fundamental Science Need:
(Derived Need)

Basic microbial, chemical, and geochemical studies are desired to support development of an in situ method for treatment of volatile organic contaminants in groundwater located in deep fracture rock environments.

Project Number:	Title	Institution:
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory

55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

Fundamental Science Need: (Derived Need) Basic biological and biochemical studies are needed to understand biological metabolism (single species and consortia) of halogenated organic compounds and metal/radionuclide organic complex in subsurface hydrogeological environments.

Project Number:	Title	Institution:
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory
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54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory

Fundamental Science Need: (Derived Need) Basic chemistry, geochemical, and fluid flow studies are needed to understand movement of contaminant (Tc, Sc, U, Cs, and Sr) through zones of low moisture and to understand the movement of water as liquid and vapor phases and retention of water on particle surfaces that improve dose calculations.

Project Number:	Title	Institution:
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory

54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory

Geochemistry

STCG Number: AL-09-01-10-SC-S Physics of Fracture Flow and Transport in the Vadose Zone **Site:** AL

Fundamental Science Need:
(STCG Science Need)

There are multiple barriers to our ability to understand and quantify the role of fractures in flow and transport in the vadose zone. One barrier is the complex geometry of the pore space of an individual fracture. Although fractures are most commonly modeled either as parallel plates (fracture network models) or high porosity - high permeability porous media (standard FEM or FDM approach), fractures are, in reality gaps of highly irregular apertures. To further complicate things, the fracture walls typically have heterogeneous mineralogy, part or all of the fracture may be coated with minerals distinct from those found in the matrix, and/or it may be blocked at points by material filling the gap. How such variability of the fracture affects flow and transport in the fracture itself, and between the fracture and the surrounding porous matrix is unknown. Another barrier to representing fracture flow and transport is in understanding the role of the interface between the fracture and matrix. Interfacial processes may strongly drive the overall flow and transport characteristics of the fracture-matrix system. Movement of fluids between fracture and matrix may occur via many processes, including advective flow, diffusion, capillary action, or vapor phase transport. How the physical characteristics of the fracture walls affects this fluid movement is not known. This lack of understanding makes incorporation of fractures, or the role of fractures, into field scale models very difficult. However, it is this leap from fundamental, detailed understanding at the fracture scale to model abstraction and incorporation into groundwater flow models that must be accomplished in order for mechanistic studies to have their greatest impact. There are a number of steps to improving our understanding of the role of fractures in movement of fluids in the vadose zone at many scales. One of the most valuable pieces of information, at our current level of understanding, is to identify the sensitivity of the fracture system to different potential variables, such as fracture surface characteristics, matrix characteristics, possible hysteretic effects during wetting or drying, etc. These sensitivity analyses can be pursued within existing numerical models. Another step in improving understanding is to study the fracture and fracture-matrix interface in detail, to quantify how fracture roughness, contact points, and surface conditions influence fracture permeability, transport between fracture and matrix, and trapping or removal of contaminants. These studies are also possible using computational models that already exist at Los Alamos. The next step is to determine the best method of incorporating our understanding of fractures and fracture flow into the field scale models that must be used if we are to study regional flow systems. Given current computational limitations, as well as fundamental limitations in the ability to characterize the pore space of a large scale system in detail, regional scale models must certainly abstract the information from more detailed studies. Therefore, an important step in the process of understanding fracture flow and transport is to integrate the information obtained in the previous steps, as well as to test the range of validity and accuracy of other approaches, such as dual porosity, discrete fracture network models, etc. Again, most of the necessary capabilities for this step are available in existing Los Alamos models. We also must rely heavily on ongoing laboratory scale experimental work being performed at Los Alamos by Reimus and at Sandia by Glass.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory

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STCG Number: AL-09-01-12-SC-S Groundwater-Surface Water Interactions **Site:** AL

Fundamental Science Need:
(STCG Science Need)

As water resources become of increasing concern, both in the U.S. and world-wide, more and more communities are turning to conjunctive use of groundwater and surface water to meet their needs. Any rational conjunctive use management requires an understanding of the effects of the interaction between groundwater and surface water, i.e., what effect does groundwater pumping have on streamflow, and what affect do surface water diversion have on groundwater recharge? Groundwater-surface water interactions has implications for water quality issues as well as water supply issues. In arid and semi-arid environments, infiltration is often the major source of uncertainty in simulations of contaminant transport in the vadose zone (e.g., Hanford, Yucca Mountain, Los Alamos). Better understanding of this term would help reduce this uncertainty. This involves better understanding of the exchange of water vapor at the air-land interface and spatial and temporal variability. The successful investigation of these interactions will require: - Field observations and experiments for input to predictive tools, and values against which to validate those models. - The appropriate surface water, vadose zone, and groundwater models to represent the conceptual model. - Better knowledge and representation of the physics at the surface.

Project Number:	Title	Institution:
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

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STCG Number: AL-09-01-14-SC-S Vadose Zone Flux Rates **Site:** AL

Fundamental Science Need:
(STCG Science Need)

Waste and contamination at many DOE sites is located in the unsaturated or vadose zone. A sensitive parameter is the flux of water moving through the vadose zone in order to estimate potential contaminant movement to the saturated zone. The highly variable input to the system from the climate, land use changes, ecological succession, and soil forming processes introduce large uncertainties in this estimate. This is particularly true for radionuclides where long-term flux estimates (periods >100 years) are needed. Performance assessment maintenance programs at operational waste sites and environmental restoration remediation decisions have a need for understanding these flux rates for the groundwater pathway component.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

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STCG Number: ID-6.1.04 In-situ Treatment of VOC Contaminated Groundwater in Deep Fractured Rock **Site:** ID

Fundamental Science Need: (Derived Need)
Basic microbial, chemical, and geochemical studies are desired to support development of an in situ method for treatment of volatile organic contaminants in groundwater located in deep fracture rock environments.

Project Number:	Title	Institution:
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory

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STCG Number: ID-S.1.07 Facilitated Transport at DOE Disposal Sites **Site:** ID

Fundamental Science Need: (STCG Science Need)
Monitoring of vadose zone and aquifer concentrations indicates the facilitated transport of radionuclides is occuring at DOE disposal and environmental remediation sites. An understanding of the mechanisms and controlling factors contributing to radionuclide facilitated transport is necessary to predict potential human health risks for these sites. Identification of the chemical form of these contaminants and the hydrologic mechanism that transports these contaminants large distances through the fractured basalts is needed.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory

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STCG Number: ID-S.1.08 Contaminant Transport in a Fractured Rock Vadose Zone **Site:** ID

Fundamental Science Need: (STCG Science Need)
Recovered rock and sediment core, soil gas sampling, soil moisture sampling and ground water sampling indicate that organic contaminants and radioactive wastes move in the vadose through discrete, preferential flowpaths driven by intermittent infiltration events. Identification and monitoring of these preferential flow paths is very difficult. Current monitoring and modeling uses a volume-averaged approach for developing conceptual and numerical models of the vadose zone based upon characterization measurements performed on discrete volumes of the subsurface. An understanding of the significance of preferential flow is needed to predict potential human health risks for these sites. Technologies, instruments and approaches are needed for characterizing and monitoring beneath several INEEL sites.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory

55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Lawrence Berkeley National Laboratory

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STCG Number: ID-S.2.03 — Aqueous Transport of Soluble Radionuclides and Heavy Metals: Evaluation of Non-Equilibrium Processes and Native Surfaces in Porous Media — **Site:** ID

Fundamental Science Need:
(STCG Science Need)

Reaction kinetics, equilibrium, and reversibility of heavy metal sorption on subsurface minerals need to be studied for site-specific, native surfaces in both long and short time frames. This is necessary to develop and improve techniques to mobilize or immobilize radioactive contaminants, and to evaluate the applicability of metal partitioning models that are based on thermodynamic equilibrium assumptions.

Project Number:	Title	Institution:
54576	On the Inclusion of the Interfacial Area Between Phases in the Physical and Mathematical Description of Subsurface Multiphase Flow	Lawrence Livermore National Laboratory
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Lawrence Berkeley National Laboratory

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STCG Number: ORHY-01a — Dense Non-Aqueous Phase Liquid (DNAPL) Source Characterization, Containment, and Treatment — **Site:** OR

Fundamental Science Need:
(Derived Need)

Basic microbial, chemical, and engineering science studies associated with characterization, and remediation of carbon tetrachloride as a dense nonaqueous phase liquid in the subsurface is needed to support closure of the Rocky Flats plant.

Project Number:	Title	Institution:
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory

Fundamental Science Need: (Derived Need)

Basic geochemical and chemical investigations are needed to understand changes to steady state chemistry of carbon tetrachloride degradation due to manipulation of subsurface conditions either by emplacement of containment materials or by addition of chemicals that alter oxidation/reduction potential of the aquifer.

Project Number:	Title	Institution:
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

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STCG Number: RL-SS25-S Chemical Form and Mobility of Dense, Non-Aqueous Phase Liquids in Hanford Subsurface Transport of **Site:** RL

Fundamental Science Need: (STCG Science Need)

Free-phase DNAPL can constitute a major secondary contaminant source so its chemical form and mobility need to be established. Science needs include the solubility and speciation of DNAPL in Hanford groundwaters, as well as the possibility of free product DNAPL. Constitutive properties (e.g. interfacial tension, entry pressure) of multiple fluids (air, water, free product DNAPL) are needed to model the form and potential mobility of DNAPLs in the subsurface. The interaction of DNAPL with mineral surfaces or with naturally occurring organic matter should be determined to gain additional information on chemical form. Key science needs on DNAPL form and mobility also include determining how NAPLs are distributed with regard to specific pore geometries and how the physical setting affects their extractability. Additional information is also needed about the role of surfactants and other agents on the basic physical properties(solubility, interfacial tensions) of NAPLs or dissolved organics and how these relations can be exploited to mobilize such contaminants. Science is also needed to extend the theoretical and computational basis for the physics of subsurface multiple phase fluid flow and transport.

Project Number:	Title	Institution:
55411	Joint Inversion of Geophysical Data for Site Characterization and Restoration Monitoring	Lawrence Livermore National Laboratory
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory

STCG Number: RL-SS26-S — Reaction Rates for Key Contaminant Species and Complexes in Site-Specific Groundwaters — **Site:** RL

Fundamental Science Need: (STCG Science Need)
Basic chemical and geochemical investigations are needed to better understand reaction rates for key contaminant species and complexes in Hanford groundwater. Information concerning in situ chemical speciation of hydroxides, carbonates, sulfates, oxyanions, and organic complexes as a function of hydrochemical condition is needed to determine how to immobilize or release contaminants.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

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STCG Number: RL-SS29-S — Effect of Subsurface Heterogeneities on Chemical Reaction and Transport — **Site:** RL

Fundamental Science Need: (STCG Science Need)
Basic geoscience, geophysical, and geochemical studies are needed to characterize physical and chemical heterogeneity using remote detection methods and to develop interpretation methods that can account for variation in sediment moisture, grain size, and clay content.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55264	High Resolution Definition of Subsurface Heterogeneity for Understanding the Biodynamics of Natural Field Systems: Advancing the Ability for Scaling to Field Conditions	Lawrence Berkeley National Laboratory

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STCG Number: RL-SS31-S — Mathematical Formulations of Chemical Reaction/Material Transport — **Site:** RL

Fundamental Science Need: (STCG Science Need)
Basic geochemistry, chemical, and biogeochemical studies are needed to determine the formulation of chemical reactions when coupled with steady-state and transient velocity field for physical transport at a variety of temporal and length scales. This is also a need for improved models for multi-component three dimensional bioreactive transport determination.

Project Number:	Title	Institution:
54576	On the Inclusion of the Interfacial Area Between Phases in the Physical and Mathematical Description of Subsurface Multiphase Flow	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory

Geophysics

STCG Number: AL-09-01-27-SC-S Long-term Monitoring Sensor Technology **Site:** AL

Fundamental Science Need:
(STCG Science Need)

Monitoring of environmental legacy sites will be required for a 30 to 100 year period after completion of initial characterization and remediation actions. A science foundation is needed that can support the development of new and innovative sensor systems that can significantly decrease the cost as well as improve performance of this long-term environmental surveillance and monitoring requirement. Background: Commitments to continued site monitoring are typically made to regulators during negotiations on the completion of remediation activities and legacy site closure. These commitments to monitoring extend for periods of time ranging from 30 to 100 years. The intent of long-term surveillance and monitoring is to verify that remediation efforts have met site goals and that no unexpected contaminant releases have occurred. For some sites, the cost of long-term monitoring over decades can equal or exceed the original remediation cost. Science Gaps: The scientific basis to create and gain acceptance of innovative sensors needs to be significantly enhanced. Specifically, sensors to measure in situ contaminants (radionuclides, organics, and metals), geophysical, and geo-hydraulic properties and to provide real-time information are needed.

Project Number:	Title	Institution:
60141	Gamma Ray Imaging for Environmental Remediation	Lawrence Berkeley National Laboratory

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STCG Number: ID-6.1.01 In-Situ Debris Characterization for Partial Retrieval **Site:** ID

Fundamental Science Need:
(Derived Need)

Basic geophysical, physics, chemical, and instrumental studies are needed to develop improved in situ analytical determination of hazardous species associated with buried debris waste forms.

Project Number:	Title	Institution:
60141	Gamma Ray Imaging for Environmental Remediation	Lawrence Berkeley National Laboratory
65015	Three-Dimensional Positron-Sensitive Germanium Detectors	Lawrence Berkeley National Laboratory

STCG Number: ID-S.1.08 Contaminant Transport in a Fractured Rock Vadose Zone **Site:** ID

Fundamental Science Need: (STCG Science Need)

Recovered rock and sediment core, soil gas sampling, soil moisture sampling and ground water sampling indicate that organic contaminants and radioactive wastes move in the vadose through discrete, preferential flowpaths driven by intermittent infiltration events. Identification and monitoring of these preferential flow paths is very difficult. Current monitoring and modeling uses a volume-averaged approach for developing conceptual and numerical models of the vadose zone based upon characterization measurements performed on discrete volumes of the subsurface. An understanding of the significance of preferential flow is needed to predict potential human health risks for these sites. Technologies, instruments and approaches are needed for characterizing and monitoring beneath several INEEL sites.

Project Number:	Title	Institution:
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Lawrence Berkeley National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory

STCG Number: ID-S.2.03 Aqueous Transport of Soluble Radionuclides and Heavy Metals: Evaluation of Non-Equilibrium Processes and Native Surfaces in Porous Media **Site:** ID

Fundamental Science Need: (STCG Science Need)

Reaction kinetics, equilibrium, and reversibility of heavy metal sorption on subsurface minerals need to be studied for site-specific, native surfaces in both long and short time frames. This is necessary to develop and improve techniques to mobilize or immobilize radioactive contaminants, and to evaluate the applicability of metal partitioning models that are based on thermodynamic equilibrium assumptions.

Project Number:	Title	Institution:
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Lawrence Berkeley National Laboratory
54576	On the Inclusion of the Interfacial Area Between Phases in the Physical and Mathematical Description of Subsurface Multiphase Flow	Lawrence Livermore National Laboratory

STCG Number: NV18-9902-04S — Long-Term Monitoring of Upward and Downward Pathways in the Vadose Zone and Closure Caps — **Site:** NV

Fundamental Science Need: (STCG Science Need)

Monitoring of low-level waste disposal and mixed waste sites is a requirement for meeting DOE Order 5820.2A and RCRA regulations, respectively. Efficient vadose zone monitoring systems capable of responding to regulatory requirements need to be designed, demonstrated, and deployed at the radioactive waste management sites. These systems need to provide early warning of the potential for or a measurable increase in the rates of transport of waste radionuclides along transport pathways. Additionally, they need to provide data to reduce uncertainty and test conceptual models and assumptions and parameters in performance assessment studies. Optimization of instrument packages, deployment geometry, and detection capability for the NTS setting is needed. A proposal to deploy a monolayer-ET cover on an Area 3 waste cell is planned under the ASTD program.

Project Number:	Title	Institution:
60328	High Frequency Electromagnetic Impedance Measurements for Characterization, Monitoring and Verification	Lawrence Berkeley National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory
55264	High Resolution Definition of Subsurface Heterogeneity for Understanding the Biodynamics of Natural Field Systems: Advancing the Ability for Scaling to Field Conditions	Lawrence Berkeley National Laboratory
55411	Joint Inversion of Geophysical Data for Site Characterization and Restoration Monitoring	Lawrence Livermore National Laboratory

STCG Number: OK99-20 — Innovative Technology to Investigate Geology and Groundwater Flow Characteristics in Fractured Rock — **Site:** OK

Fundamental Science Need: (Derived Need)

Fundamental geoscience, hydrology, and fluid flow studies are desired to understand groundwater flow through fractured rock.

Project Number:	Title	Institution:
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory

STCG Number: ORHY-01a — Dense Non-Aqueous Phase Liquid (DNAPL) Source Characterization, Containment, and Treatment — **Site:** OR

Fundamental Science Need: (Derived Need)
Basic microbial, chemical, and engineering science studies associated with characterization, and remediation of carbon tetrachloride as a dense nonaqueous phase liquid in the subsurface is needed to support closure of the Rocky Flats plant.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory

Fundamental Science Need: (Derived Need)
Basic geochemical and chemical investigations are needed to understand changes to steady state chemistry of carbon tetrachloride degradation due to manipulation of subsurface conditions either by emplacement of containment materials or by addition of chemicals that alter oxidation/reduction potential of the aquifer.

Project Number:	Title	Institution:
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

STCG Number: RL-SS29-S — Effect of Subsurface Heterogeneities on Chemical Reaction and Transport — **Site:** RL

Fundamental Science Need: (STCG Science Need) Basic geoscience, geophysical, and geochemical studies are needed to characterize physical and chemical heterogeneity using remote detection methods and to develop interpretation methods that can account for variation in sediment moisture, grain size, and clay content.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55264	High Resolution Definition of Subsurface Heterogeneity for Understanding the Biodynamics of Natural Field Systems: Advancing the Ability for Scaling to Field Conditions	Lawrence Berkeley National Laboratory

STCG Number: RL-SS31-S — Mathematical Formulations of Chemical Reaction/Material Transport — **Site:** RL

Fundamental Science Need: (STCG Science Need) Basic geochemistry, chemical, and biogeochemical studies are needed to determine the formulation of chemical reactions when coupled with steady-state and transient velocity field for physical transport at a variety of temporal and length scales. This is also a need for improved models for multi-component three dimensional bioreactive transport determination.

Project Number:	Title	Institution:
54576	On the Inclusion of the Interfacial Area Between Phases in the Physical and Mathematical Description of Subsurface Multiphase Flow	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory

Health Science

STCG Number: AL-09-01-03-SC-S Succession and Long-Term Performance of Landfill Covers **Site:** AL

Fundamental Science Need: (STCG Science Need)

The vast majority of contamination at DOE sites will be left in situ and stabilized with an engineered landfill cover. Although many studies have evaluated the initial performance of landfill cover designs over a few years, lacking are studies that determine the long-term integrity of covers and how they will change with plant succession and associated processes. Field studies of succession and use of natural analogs for determining the long-term performance of landfill covers are needed, as called for at the December 1998 special section on Landfill Covers at the American Geophysical Union meeting. Further, modeling that integrates hydrology of covers, succession, and risk is totally lacking and needed to address this problem.

Project Number:	Title	Institution:
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

Hydrogeology

STCG Number: AL-09-01-01-SC-S Transport of HE and Metals in Fractured Rock and Surface Alluvial Systems **Site:** AL

Fundamental Science Need: (STCG Science Need)

Los Alamos National Laboratory's Technical Area (TA) 16 contains multiple sites contaminated with high concentrations of high explosives (HE), particularly RDX, and metals, particularly barium. TA-16 springs, perched groundwaters, and surface waters are contaminated with HE and barium at levels of regulatory concern. Because HE and metal constituents will probably be left 'in place', both in the vadose zone and in the alluvial system, a science-based understanding of fate and transport of HE and metals in these media is vital. Specific questions that need to be addressed using a science-based approach include: ? How to delineate and understand subsurface transport pathways in a heterogeneous, fractured vadose zone? ? How to best identify recharge sources and discharge sinks for contaminated waters? ? How to define the nature, timing, and dynamics of contaminant transport in surface alluvial systems? ? How to define connectivity between individual contaminated sites and contaminated waters in the alluvial system and in the subsurface? ? How do all of these constituents affect ecological receptors? Answering these questions can be used to develop and refine validated numerical models for contaminant transport – both in the fractured vadose zone and in alluvial systems. Answering these questions can also help DOE defend remedial alternatives that include monitored natural attenuation and\or leaving waste in place.

Project Number:	Title	Institution:
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory

STCG Number: AL-09-01-03-SC-S Succession and Long-Term Performance of Landfill Covers **Site:** AL

Fundamental Science Need:
(STCG Science Need)

The vast majority of contamination at DOE sites will be left in situ and stabilized with an engineered landfill cover. Although many studies have evaluated the initial performance of landfill cover designs over a few years, lacking are studies that determine the long-term integrity of covers and how they will change with plant succession and associated processes. Field studies of succession and use of natural analogs for determining the long-term performance of landfill covers are needed, as called for at the December 1998 special section on Landfill Covers at the American Geophysical Union meeting. Further, modeling that integrates hydrology of covers, succession, and risk is totally lacking and needed to address this problem.

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55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

STCG Number: AL-09-01-06-SC-S Issue of Scale in Flow Prediction and Contaminant Remediation in Porous Media **Site:** AL

Fundamental Science Need:
(STCG Science Need)

Flow and transport in the subsurface is influenced by processes and interactions that occur across vastly different length scales. The characteristics of the pore space itself determines where fluids move and where fluids are trapped. Larger scale heterogeneities influence the extent of dispersion, and first arrival times. Traditional methods of modeling and predicting such flow and transport are also subject to issues of scale. Flow characteristics are measured in the laboratory on samples that range from around 2 cm to 30 cm in length. These samples may be taken from field locations that are spaced from tens to hundreds of meters apart. They may be utilized in models to represent grid blocks of meters to hundreds of meters. The objective may be to model a system that spans many square kilometers. The governing equations that are used to describe flow and transport in groundwater systems are also subject to scaling issues. Traditional modeling approaches use volume averaged equations (e.g. Darcy´s Law). However, standard Darcian techniques inherently mask fine scale (i.e. pore) details through the averaging process, and depend on small scale (i.e. laboratory) to represent much larger (grid block) scales. We are increasingly aware that contaminant remediation and predictive applications are severely limited by our lack of understanding of the functional relationship between aquifer scale flow, the volume averaged parameters used, and the microscopic processes occurring at the pore scale. The solution to this problem lies in identifying and quantifying what information must be transferred from one scale to another, and determining the most accurate and efficient means for moving such information between scales. There are a number of potential techniques for upscaling of information. We at Los Alamos have expertise in the question of scaling and are developing scaling methods that are currently being applied and tested on the oil and gas recovery problem, which is a direct analog of the groundwater flow and remediation question. The end result will be an ability to predict flow and transport in the subsurface that is closely linked to the actual physical processes that affect fluid movement, thus reducing (though not eliminating) the uncertainty of the results.

Project Number:	Title	Institution:
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous	Lawrence Livermore National Laboratory

Vadose Regimes

STCG Number: AL-09-01-08-SC-S Differences Between Saturated and Unsaturated Systems **Site:** AL

Fundamental Science Need:
(STCG Science Need)

The numerical representation of transport in the unsaturated zone is adapted from transport methods developed for saturated systems. However, as the water content changes, there has been experimental evidence that dispersion and other common parameters used in numerical modeling may have a non-linear relationship as a function of saturation. This indicates that parameters used for saturated modeling may not be scalable to unsaturated systems and that other processes may need to be considered. Defining the correct transport parameters requires a combined effort between laboratory and field experiments, and computational modeling. Intermediate scale laboratory experiments must be used to determine appropriate unsaturated transport parameters that can then be used to improve the parameter representation in the model for general classes of contaminants, such as radionuclides, hydrocarbons, and heavy metals. This area of research applies to both porous media and fractured rock. Although both will need to be addressed, it is most important to initially focus on porous media until there is a better foundation for flow and transport processes in fractured rock.

Project Number:	Title	Institution:
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
54576	On the Inclusion of the Interfacial Area Between Phases in the Physical and Mathematical Description of Subsurface Multiphase Flow	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

STCG Number: AL-09-01-10-SC-S Physics of Fracture Flow and Transport in the Vadose Zone **Site:** AL

Fundamental Science Need:
(STCG Science Need)

There are multiple barriers to our ability to understand and quantify the role of fractures in flow and transport in the vadose zone. One barrier is the complex geometry of the pore space of an individual fracture. Although fractures are most commonly modeled either as parallel plates (fracture network models) or high porosity - high permeability porous media (standard FEM or FDM approach), fractures are, in reality gaps of highly irregular apertures. To further complicate things, the fracture walls typically have heterogeneous mineralogy, part or all of the fracture may be coated with minerals distinct from those found in the matrix, and/or it may be blocked at points by material filling the gap. How such variability of the fracture affects flow and transport in the fracture itself, and between the fracture and the surrounding porous matrix is unknown. Another barrier to representing fracture flow and transport is in understanding the role of the interface between the fracture and matrix. Interfacial processes may strongly drive the overall flow and transport characteristics of the fracture-matrix system. Movement of fluids between fracture and matrix may occur via many processes, including advective flow, diffusion, capillary action, or vapor phase transport. How the physical characteristics of the fracture walls affects this fluid movement is not known. This lack of understanding makes incorporation of fractures, or the role of fractures, into field scale models very difficult. However, it is this leap from fundamental, detailed understanding at the fracture scale to model abstraction and incorporation into groundwater flow models that must be accomplished in order for mechanistic studies to have their greatest impact. There are a number of steps to improving our understanding of the role of fractures in movement of fluids in the vadose zone at many scales. One of the most valuable pieces of information, at our current level of understanding, is to identify the sensitivity of the fracture system to different potential variables, such as fracture surface characteristics, matrix characteristics, possible hysteretic effects during wetting or drying, etc. These sensitivity analyses can be pursued within existing numerical models. Another step in improving understanding is to study the fracture and fracture-matrix interface in detail, to quantify how fracture roughness, contact points, and surface conditions influence fracture permeability, transport between fracture and matrix, and trapping or removal of contaminants. These studies are also possible using computational models that already exist at Los Alamos. The next step is to determine the best method of incorporating our understanding of fractures and fracture flow into the field scale models that must be used if we are to study regional flow systems. Given current computational limitations, as well as fundamental limitations in the ability to characterize the pore space of a large scale system in detail, regional scale models must certainly abstract the information from more detailed studies. Therefore, an important step in the process of understanding fracture flow and transport is to integrate the information obtained in the previous steps, as well as to test the range of validity and accuracy of other approaches, such as dual porosity, discrete fracture network models, etc. Again, most of the necessary capabilities for this step are available in existing Los Alamos models. We also must rely heavily on ongoing laboratory scale experimental work being performed at Los Alamos by Reimus and at Sandia by Glass.

Project Number:	Title	Institution:
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

STCG Number: AL-09-01-11-SC-S Water Fluxes and Solute Transport in Arid and Semiarid Environments **Site:** AL

Fundamental Science Need:
(STCG Science Need)

The hydrology of arid and semiarid regions of the American West and worldwide is becoming increasingly important both for water resources and environmental protection issues. As the sun-belt population soars, water resource demands are increasing, and more and more urban areas are seeking external sources of groundwater, often from desert basins. Both regulatory drivers and common sense require quantification of the long-term sustainable yield of these basins before reasonable political decisions on the appropriateness of such water transfers can be made. This quantification, in turn, requires a scientific understanding of arid-zone recharge processes. At the same time, society is turning to arid regions for disposal of long-lived wastes, both radioactive and chemical. This trend is being driven by the reasonable assumption that the low recharge fluxes and thick vadose zones of desert regions will provide a natural barrier between the waste and the accessible environment. Society, through its regulatory agencies, demands quantification of the degree of protection afforded by this natural barrier. Infiltration is often the major source of uncertainty in simulations of flow and transport in the vadose zone in arid and semi-arid environments. Quantification hinges on a scientific understanding of the exchange of water vapor at the air-land interface and spatial and temporal variability. Currently our understanding is limited by lack of knowledge in a variety of areas, including: - Hydraulic behavior of very dry porous and fractured media - Effects of strong transient thermal and matric gradients - Vadose-zone / atmospheric interactions - Significance of vapor-phase water fluxes - Possible net evaporation from deep water tables These and other important research areas can best be addressed by a multidisciplinary effort incorporating: - Field observations and experiments (including tracer tests) - Laboratory-scale column experiments - Numerical modeling studies - Theoretical studies in soil physics

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory

STCG Number: AL-09-01-12-SC-S Groundwater-Surface Water Interactions **Site:** AL

Fundamental Science Need:
(STCG Science Need)

As water resources become of increasing concern, both in the U.S. and world-wide, more and more communities are turning to conjunctive use of groundwater and surface water to meet their needs. Any rational conjunctive use management requires an understanding of the effects of the interaction between groundwater and surface water, i.e., what effect does groundwater pumping have on streamflow, and what affect do surface water diversion have on groundwater recharge? Groundwater-surface water interactions has implications for water quality issues as well as water supply issues. In arid and semi-arid environments, infiltration is often the major source of uncertainty in simulations of contaminant transport in the vadose zone (e.g., Hanford, Yucca Mountain, Los Alamos). Better understanding of this term would help reduce this uncertainty. This involves better understanding of the exchange of water vapor at the air-land interface and spatial and temporal variability. The successful investigation of these interactions will require: - Field observations and experiments for input to predictive tools, and values against which to validate those models. - The appropriate surface water, vadose zone, and groundwater models to represent the conceptual model. - Better knowledge and representation of the physics at the interface.

Project Number:	Title	Institution:
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

STCG Number: AL-09-01-14-SC-S Vadose Zone Flux Rates **Site:** AL

Fundamental Science Need:
(STCG Science Need)

Waste and contamination at many DOE sites is located in the unsaturated or vadose zone. A sensitive parameter is the flux of water moving through the vadose zone in order to estimate potential contaminant movement to the saturated zone. The highly variable input to the system from the climate, land use changes, ecological succession, and soil forming processes introduce large uncertainties in this estimate. This is particularly true for radionuclides where long-term flux estimates (periods >100 years) are needed. Performance assessment maintenance programs at operational waste sites and environmental restoration remediation decisions have a need for understanding these flux rates for the groundwater pathway component.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

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STCG Number: AL-09-01-27-SC-S Long-term Monitoring Sensor Technology **Site:** AL

Fundamental Science Need:
(STCG Science Need)

Monitoring of environmental legacy sites will be required for a 30 to 100 year period after completion of initial characterization and remediation actions. A science foundation is needed that can support the development of new and innovative sensor systems that can significantly decrease the cost as well as improve performance of this long-term environmental surveillance and monitoring requirement. Background: Commitments to continued site monitoring are typically made to regulators during negotiations on the completion of remediation activities and legacy site closure. These commitments to monitoring extend for periods of time ranging from 30 to 100 years. The intent of long-term surveillance and monitoring is to verify that remediation efforts have met site goals and that no unexpected contaminant releases have occurred. For some sites, the cost of long-term monitoring over decades can equal or exceed the original remediation cost. Science Gaps: The scientific basis to create and gain acceptance of innovative sensors needs to be significantly enhanced. Specifically, sensors to measure in situ contaminants (radionuclides, organics, and metals), geophysical, and geo-hydraulic properties and to provide real-time information as needed.

Project Number:	Title	Institution:
60141	Gamma Ray Imaging for Environmental Remediation	Lawrence Berkeley National Laboratory

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STCG Number: ID-S.1.07 Facilitated Transport at DOE Disposal Sites **Site:** ID

Fundamental Science Need:
(STCG Science Need)

Monitoring of vadose zone and aquifer concentrations indicates the facilitated transport of radionuclides is occuring at DOE disposal and environmental remediation sites. An understanding of the mechanisms and controlling factors contributing to radionuclide facilitated transport is necessary to predict potential human health risks for these sites. Identification of the chemical form of these contaminants and the hydrologic mechanism that transports these contaminants large distances through the fractured basalts is needed.

Project Number:	Title	Institution:
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

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STCG Number: ID-S.1.08 Contaminant Transport in a Fractured Rock Vadose Zone **Site:** ID

Fundamental Science Need: (STCG Science Need)

Recovered rock and sediment core, soil gas sampling, soil moisture sampling and ground water sampling indicate that organic contaminants and radioactive wastes move in the vadose through discrete, preferential flowpaths driven by intermittent infiltration events. Identification and monitoring of these preferential flow paths is very difficult. Current monitoring and modeling uses a volume-averaged approach for developing conceptual and numerical models of the vadose zone based upon characterization measurements performed on discrete volumes of the subsurface. An understanding of the significance of preferential flow is needed to predict potential human health risks for these sites. Technologies, instruments and approaches are needed for characterizing and monitoring beneath several INEEL sites.

Project Number:	Title	Institution:
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Lawrence Berkeley National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

STCG Number: ID-S.2.01 Definition of ´Biologically Active Zones´ in Fractured Rock Environments **Site:** ID

Fundamental Science Need: (STCG Science Need)

Fundamental understanding of biogeochemical reactions (including rates and extents) with contaminants in the subsurface as they are related to specific conditions (e.g. fractures, rubble zones, interbeds) such that biologically active zones can be predicted and evaluated more effectively.

Project Number:	Title	Institution:
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory
54698	Rapid Mass Spectrometric DNA Diagnostics for Assessing Microbial Community Activity During Bioremediation	Lawrence Berkeley National Laboratory

STCG Number: OK99-20 — Innovative Technology to Investigate Geology and Groundwater Flow Characteristics in Fractured Rock — **Site:** OK

Fundamental Science Need: (Derived Need) Fundamental geoscience, hydrology, and fluid flow studies are desired to understand groundwater flow through fractured rock.

Project Number:	Title	Institution:
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

Inorganic Chemistry

STCG Number: CH-SS01-99 — Remediation of Strontium-90 Contaminated Groundwater — **Site:** CH

Fundamental Science Need: (Derived Need) Fundamental inorganic and separations chemistry are needed to support remediation of Strontium-90 in groundwater.

Project Number:	Title	Institution:
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory

STCG Number: ORHY-12a — Active In Situ Dissolved Phase Treatment Systems — **Site:** OR

Fundamental Science Need: (Derived Need) Fundamental study of reacting flows in heterogeneous porous media, heat transfer, chemistry, microbial and engineering sciences are needed to support efforts to develop technologies for in situ remediation of high explosives, solvents, volatile organic compounds, semi-volatile organic compounds, heavy metals, and landfill materials.

Project Number:	Title	Institution:
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution	Lawrence Livermore National Laboratory

	Chemistry	
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory

Fundamental Science Need: (Derived Need)

Basic microbial, chemical, and geochemical studies are desired to support development of an in situ method for treatment of volatile organic contaminants in groundwater located in deep fracture rock environments.

Project Number:	Title	Institution:
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory

Fundamental Science Need: (Derived Need)

Basic biological and biochemical studies are needed to understand biological metabolism (single species and consortia) of halogenated organic compounds and metal/radionuclide organic complex in subsurface hydrogeological environments.

Project Number:	Title	Institution:
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory

55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

Fundamental Science Need:
(Derived Need)

Basic chemistry, geochemical, and fluid flow studies are needed to understand movement of contaminant (Tc, Sc, U, Cs, and Sr) through zones of low moisture and to understand the movement of water as liquid and vapor phases and retention of water on particle surfaces that improve dose calculations.

Project Number:	Title	Institution:
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory

`STCG Number: RL-SS25-S Chemical Form and Mobility of Dense, Non-Aqueous Phase Liquids in Hanford Subsurface Transport of Contaminants **Site:** RL

Fundamental Science Need: (STCG Science Need)

Free-phase DNAPL can constitute a major secondary contaminant source so its chemical form and mobility need to be established. Science needs include the solubility and speciation of DNAPL in Hanford groundwaters, as well as the possibility of free product DNAPL. Constitutive properties (e.g. interfacial tension, entry pressure) of multiple fluids (air, water, free product DNAPL) are needed to model the form and potential mobility of DNAPLs in the subsurface. The interaction of DNAPL with mineral surfaces or with naturally occurring organic matter should be determined to gain additional information on chemical form. Key science needs on DNAPL form and mobility also include determining how NAPLs are distributed with regard to specific pore geometries and how the physical setting affects their extractability. Additional information is also needed about the role of surfactants and other agents on the basic physical properties (solubility, interfacial tensions) of NAPLs or dissolved organics and how these relations can be exploited to mobilize such contaminants. Science is also needed to extend the theoretical and computational basis for the physics of subsurface multiple phase fluid flow and transport.

Project Number:	Title	Institution:
55411	Joint Inversion of Geophysical Data for Site Characterization and Restoration Monitoring	Lawrence Livermore National Laboratory
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory

Materials Science

STCG Number: ID-S.1.07 Facilitated Transport at DOE Disposal Sites **Site:** ID

Fundamental Science Need: (STCG Science Need)

Monitoring of vadose zone and aquifer concentrations indicates the facilitated transport of radionuclides is occuring at DOE disposal and environmental remediation sites. An understanding of the mechanisms and controlling factors contributing to radionuclide facilitated transport is necessary to predict potential human health risks for these sites. Identification of the chemical form of these contaminants and the hydrologic mechanism that transports these contaminants large distances through the fractured basalts is needed.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory

STCG Number: ORHY-12a Active In Situ Dissolved Phase Treatment Systems **Site:** OR

Fundamental Science Need: (Derived Need)
Fundamental study of reacting flows in heterogeneous porous media, heat transfer, chemistry, microbial and engineering sciences are needed to support efforts to develop technologies for in situ remediation of high explosives, solvents, volatile organic compounds, semi-volatile organic compounds, heavy metals, and landfill materials.

Project Number:	Title	Institution:
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory

Fundamental Science Need: (Derived Need)
Basic microbial, chemical, and geochemical studies are desired to support development of an in situ method for treatment of volatile organic contaminants in groundwater located in deep fracture rock environments.

Project Number:	Title	Institution:
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

Fundamental Science Need: (Derived Need)

Basic biological and biochemical studies are needed to understand biological metabolism (single species and consortia) of halogenated organic compounds and metal/radionuclide organic complex in subsurface hydrogeological environments.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory

Fundamental Science Need: (Derived Need)

Basic chemistry, geochemical, and fluid flow studies are needed to understand movement of contaminant (Tc, Sc, U, Cs, and Sr) through zones of low moisture and to understand the movement of water as liquid and vapor phases and retention of water on particle surfaces that improve dose calculations.

Project Number:	Title	Institution:
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

STCG Number: RL-SS29-S — Effect of Subsurface Heterogeneities on Chemical Reaction and Transport — **Site:** RL

Fundamental Science Need: (STCG Science Need)
Basic geoscience, geophysical, and geochemical studies are needed to characterize physical and chemical heterogeneity using remote detection methods and to develop interpretation methods that can account for variation in sediment moisture, grain size, and clay content.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55264	High Resolution Definition of Subsurface Heterogeneity for Understanding the Biodynamics of Natural Field Systems: Advancing the Ability for Scaling to Field Conditions	Lawrence Berkeley National Laboratory

Plant Science

STCG Number: AL-07-04-01-SC — Non-Itrusive Removal of Polychlorinated Biphenols (PCBs) from Soil Both Above and Below the Water Table Underneath Buildings — **Site:** AL

Fundamental Science Need: (Derived Need)
Chemical and microbial science studies are needed to support non-intrusive removal of polychlorinated biphenol from soils located underneath buildings

Project Number:	Title	Institution:
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Lawrence Berkeley National Laboratory

STCG Number: AL-07-06-04-SC — In Situ Remediation Of HE, Solvents, VOCs, SVOCs, Heavy Metals, And Landfill Materials — **Site:** AL

Fundamental Science Need: (Derived Need)
Fundamental study of reacting flows in heterogeneous porous media, heat transfer, chemistry, microbial and engineering sciences are needed to support efforts to develop technologies for in situ remediation of high explosives, solvents, volatile organic compounds, semi-volatile organic compounds, heavy metals, and landfill materials.

Project Number:	Title	Institution:
55343	Enzyme Engineering for Biodegradation of Chlorinated Organic Pollutants	Lawrence Berkeley National Laboratory
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Lawrence Berkeley National Laboratory

STCG Number: ORHY-01a Dense Non-Aqueous Phase Liquid (DNAPL) Source Characterization, Containment, and Treatment **Site:** OR

Fundamental Science Need: (Derived Need) Basic microbial, chemical, and engineering science studies associated with characterization, and remediation of carbon tetrachloride as a dense nonaqueous phase liquid in the subsurface is needed to support closure of the Rocky Flats plant.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory

Fundamental Science Need: (Derived Need) Basic geochemical and chemical investigations are needed to understand changes to steady state chemistry of carbon tetrachloride degradation due to manipulation of subsurface conditions either by emplacement of containment materials or by addition of chemicals that alter oxidation/reduction potential of the aquifer.

Project Number:	Title	Institution:
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55011	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes	Lawrence Livermore National Laboratory
55351	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL	Lawrence Berkeley National Laboratory

Separations Chemistry

STCG Number: AL-07-04-01-SC — Non-Itrusive Removal of Polychlorinated Biphenols (PCBs) from Soil Both Above and Below the Water Table Underneath Buildings — **Site:** AL

Fundamental Science Need: (Derived Need)
Chemical and microbial science studies are needed to support non-intrusive removal of polychlorinated biphenol from soils located underneath buildings.

Project Number:	Title	Institution:
55396	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology	Lawrence Berkeley National Laboratory

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STCG Number: CH-SS01-99 — Remediation of Strontium-90 Contaminated Groundwater — **Site:** CH

Fundamental Science Need: (Derived Need)
Fundamental inorganic and separations chemistry are needed to support remediation of Strontium-90 in groundwater.

Project Number:	Title	Institution:
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory

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STCG Number: ORHY-12a — Active In Situ Dissolved Phase Treatment Systems — **Site:** OR

Fundamental Science Need: (Derived Need)
Fundamental study of reacting flows in heterogeneous porous media, heat transfer, chemistry, microbial and engineering sciences are needed to support efforts to develop technologies for in situ remediation of high explosives, solvents, volatile organic compounds, semi-volatile organic compounds, heavy metals, and landfill materials.

Project Number:	Title	Institution:
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory

55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory

Fundamental Science Need:
(Derived Need)

Basic microbial, chemical, and geochemical studies are desired to support development of an in situ method for treatment of volatile organic contaminants in groundwater located in deep fracture rock environments.

Project Number:	Title	Institution:
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory

Fundamental Science Need:
(Derived Need)

Basic biological and biochemical studies are needed to understand biological metabolism (single species and consortia) of halogenated organic compounds and metal/radionuclide organic complex in subsurface hydrogeological environments.

Project Number:	Title	Institution:
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

Subsurface Contaminants Focus Area
Associated Research Needs and EMSP Projects

Fundamental Science Need: (Derived Need)

Basic chemistry, geochemical, and fluid flow studies are needed to understand movement of contaminant (Tc, Sc, U, Cs, and Sr) through zones of low moisture and to understand the movement of water as liquid and vapor phases and retention of water on particle surfaces that improve dose calculations.

Project Number:	Title	Institution:
60041	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
55249	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory

Actinide Chemistry

STCG Number: RL-WT041-S Radionuclide Partitioning **Site:** RL

Fundamental Science Need: (STCG Science Need)
Chemical and engineering science studies are needed to understand, determine, or predict the partitioning of important radionuclides (especially Tc-99) among the waste processing solutions, suspended solids, and precipitates in these high ionic strength solutions so that efficient waste processes can be developed to reduce the volume of high level waste treated.

Project Number:	Title	Institution:
65352	Developing a Fundamental Basis for the Characterization, Separation, and Disposal of Plutonium and Other Actinides in High Level Radioactive Waste: The Effect of Temperature and Electrolyte Concentrations on Actinide Speciation	Lawrence Berkeley National Laboratory
60296	Research Program to Investigate the Fundamental Chemistry of Technetium	Lawrence Berkeley National Laboratory
65398	Characterization of Actinides in Simulated Alkaline Tank Waste Sludges and Leach Solutions	Lawrence Berkeley National Laboratory

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STCG Number: RL-WT048-S Inovative Methods for Radionuclide Separation **Site:** RL

Fundamental Science Need: (STCG Science Need)
Fundamental chemical science investigations of the speciation of technetium and strontium are needed to develop process and techniques to remove these materials and reduce the volume of high and low level waste.

Project Number:	Title	Institution:
65352	Developing a Fundamental Basis for the Characterization, Separation, and Disposal of Plutonium and Other Actinides in High Level Radioactive Waste: The Effect of Temperature and Electrolyte Concentrations on Actinide Speciation	Lawrence Berkeley National Laboratory
65368	Speciation, inauguration, and Redox Reactions of Chromium Relevant to Pretreatment and Separation of High-Level Tank Wastes	Lawrence Berkeley National Laboratory
65370	Actinide-Specific Interfacial Chemistry of Monolayer Coated Mesoporous Ceramics	Lawrence Berkeley National Laboratory

Engineering Sciences

STCG Number: RL-WT042-S Flammable Gas Generation, Retention, and Release in HLW Tanks **Site:** RL

Fundamental Science Need: (STCG Science Need)
Basic chemical and engineering science studies are needed to understand high level waste gas release mechanisms, such as bubble movement or gas diffusion, for different waste types and configurations so that flammable gas release rate from high level waste in tanks can be estimated.

Project Number:	Title	Institution:
60451	Mechanics of Bubbles in Sludges and Slurries	Lawrence Berkeley National Laboratory

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STCG Number: RL-WT049-S Effect of Processing on Waste Rheological and Sedimentation Properties **Site:** RL

Fundamental Science Need: (STCG Science Need)
Basic engineering science activities are needed to develop models that predict gel formation in processed high level waste streams and that considers rhelological properties of the waste, colloid behavior and flocculation, particle size, surface charge and interfacial properties, and mechanical mixing to predict gel formation in retrieval, wash, and leach solutions.

Project Number:	Title	Institution:
65352	Developing a Fundamental Basis for the Characterization, Separation, and Disposal of Plutonium and Other Actinides in High Level Radioactive Waste: The Effect of Temperature and Electrolyte Concentrations on Actinide Speciation	Lawrence Berkeley National Laboratory
65368	Speciation, Dissolution, and Redox Reactions of Chromium Relevant to Pretreatment and Separation of High-Level Tank Wastes	Lawrence Berkeley National Laboratory

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STCG Number: RL-WT051-S Foam Generation and Stability **Site:** RL

Fundamental Science Need: (STCG Science Need)
Fundamental engineering science investigations are needed to understand formation of foam and the stability of the foam in waste slimes is needed for understanding the transport proverties of these foams and to assess safety hazards.

Project Number:	Title	Institution:
60451	Mechanics of Bubbles in Sludges and Slurries	Lawrence Berkeley National Laboratory

Geochemistry

STCG Number: RL-WT033-S Chemistry of Problem Constituents for HLW Virtrication **Site:** RL

Fundamental Science Need: (STCG Science Need) Fundamental chemical and material science studies are needed to characterize the solution thermodynamics of multicomponent borosilicate liquids with specific focus on effects of sodium, chromium, and phosphate as a function of concentration levels.

Project Number:	Title	Institution:
60362	Ion-Exchange Processes and Mechanisms in Glasses	Lawrence Berkeley National Laboratory
60296	Research Program to Investigate the Fundamental Chemistry of Technetium	Lawrence Berkeley National Laboratory

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STCG Number: RL-WT036-S Alternate Waste Form Development **Site:** RL

Fundamental Science Need: (STCG Science Need) Basic materials science investigations are needed to understand glass and ceramic structures and phase stabilization to develop alternative waste forms for high and low-level waste. Current baseline is borosilicate.

Project Number:	Title	Institution:
60118	Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms	Lawrence Livermore National Laboratory

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STCG Number: RL-WT053-S Containment Mobility Beneath Tank Farms **Site:** RL

Fundamental Science Need: (STCG Science Need) Geoscience, geochemical, geophysical, chemical, and engineering science studies are needed to evaluation the importance of colloids in enhancing the migration of radionuclides, to characterize sorptive mechanisms of radionuclides to soil under extreme chemical conditions represented by tank effluents, and to combine known information into a computer model having temporal and spatial dependent variables with built-in degrees of uncertainty. This understanding and predictive ability is needed to characterize spread of contamination from leaking high level waste tanks.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured	Lawrence Berkeley National Laboratory

Vadose Zone

Geophysics

STCG Number: RL-WT035-S Moisture Flow and Contaminant Transport in Arid Conditions **Site:** RL

Fundamental Science Need: (STCG Science Need) Basic chemistry, geochemical, and fluid flow studies are needed to understand movement of contaminant (Tc, Sc, U, Cs, and Sr) through zones of low moisture and to understand the movement of water as liquid and vapor phases and retention of water on particle surfaces that improve dose calculations

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

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STCG Number: RL-WT045-S Vadose Zone Flow Simulation Topol Under Arid Conditions **Site:** RL

Fundamental Science Need: (STCG Science Need) Fundamental geoscience and geochemical investigations are required to develop time and spatially dependent models with transient moisture flow and contaminant transport for use in risk assessments.

Project Number:	Title	Institution:
60328	High Frequency Electromagnetic Impedance Measurements for Characterization, Monitoring and Verification	Lawrence Berkeley National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

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STCG Number: RL-WT053-S Containment Mobility Beneath Tank Farms **Site:** RL

Fundamental Science Need: (STCG Science Need) Geoscience, geochemical, geophysical, chemical, and engineering science studies are needed to evaluation the importance of colloids in enhancing the migration of radionuclides, to characterize sorptive mechanisms of radionuclides to soil under extreme chemical conditions represented by tank effluents, and to combine known information into a computer model having temporal and spatial dependent variables with built-in degrees of uncertainty. This understanding and predictive ability is needed to characterize spread of contamination from leaking high level waste tanks.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory

55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory

Hydrogeology

STCG Number: RL-WT035-S Moisture Flow and Contaminant Transport in Arid Conditions **Site:** RL

Fundamental Science Need: (STCG Science Need) Basic chemistry, geochemical, and fluid flow studies are needed to understand movement of contaminant (Tc, Sc, U, Cs, and Sr) through zones of low moisture and to understand the movement of water as liquid and vapor phases and retention of water on particle surfaces that improve dose calculations.

Project Number:	Title	Institution:
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

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60328	High Frequency Electromagnetic Impedance Measurements for Characterization, Monitoring and Verification	Lawrence Berkeley National Laboratory

Inorganic Chemistry

STCG Number: RL-WT033-S Chemistry of Problem Constituents for HLW Virtrication **Site:** RL

Fundamental Science Need: (STCG Science Need) Fundamental chemical and material science studies are needed to characterize the solution thermodynamics of multicomponent borosilicate liquids with specific focus on effects of sodium, chromium, and phosphate as a function of concentration levels.

Project Number:	Title	Institution:
60362	Ion-Exchange Processes and Mechanisms in Glasses	Lawrence Berkeley National Laboratory

60296	Research Program to Investigate the Fundamental Chemistry of Technetium	Lawrence Berkeley National Laboratory

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STCG Number: RL-WT036-S Alternate Waste Form Development **Site:** RL

Fundamental Science Need: (STCG Science Need) Basic materials science investigations are needed to understand glass and ceramic structures and phase stabilization to develop alternative waste forms for high and low-level waste. Current baseline is borosilicate.

Project Number:	Title	Institution:
60118	Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms	Lawrence Livermore National Laboratory

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STCG Number: RL-WT041-S Radionuclide Partitioning **Site:** RL

Fundamental Science Need: (STCG Science Need) Chemical and engineering science studies are needed to understand, determine, or predict the partitioning of important radionuclides (especially Tc-99) among the waste processing solutions, suspended solids, and precipitates in these high ionic strength solutions so that efficient waste processes can be developed to reduce the volume of high level waste treated.

Project Number:	Title	Institution:
60296	Research Program to Investigate the Fundamental Chemistry of Technetium	Lawrence Berkeley National Laboratory
65352	Developing a Fundamental Basis for the Characterization, Separation, and Disposal of Plutonium and Other Actinides in High Level Radioactive Waste: The Effect of Temperature and Electrolyte Concentrations on Actinide Speciation	Lawrence Berkeley National Laboratory
65398	Characterization of Actinides in Simulated Alkaline Tank Waste Sludges and Leach Solutions	Lawrence Berkeley National Laboratory

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STCG Number: RL-WT042-S Flammable Gas Generation, Retention, and Release in HLW Tanks **Site:** RL

Fundamental Science Need: (STCG Science Need) Basic chemical and engineering science studies are needed to understand high level waste gas release mechanisms, such as bubble movement or gas diffusion, for different waste types and configurations so that flammable gas release rate from high level waste in tanks can be estimated.

Project Number:	Title	Institution:
60451	Mechanics of Bubbles in Sludges and Slurries	Lawrence Berkeley National Laboratory

STCG Number: RL-WT046-S Getter Materials **Site:** RL

Fundamental Science Need: (STCG Science Need)
Basic chemical, geochemical, and geoscience studies are desired to better understand binding of negatively charged elements and compounds with soil so that appropriate materials to retard transport of these chemicals can be determined.

Project Number:	Title	Institution:
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory

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STCG Number: RL-WT048-S Inovative Methods for Radionuclide Separation **Site:** RL

Fundamental Science Need: (STCG Science Need)
Fundamental chemical science investigations of the speciation of technetium and strontium are needed to develop process and techniques to remove these materials and reduce the volume of high and low level waste.

Project Number:	Title	Institution:
65370	Actinide-Specific Interfacial Chemistry of Monolayer Coated Mesoporous Ceramics	Lawrence Berkeley National Laboratory
65368	Speciation, Dissolution, and Redox Reactions of Chromium Relevant to Pretreatment and Separation of High-Level Tank Wastes	Lawrence Berkeley National Laboratory
65352	Developing a Fundamental Basis for the Characterization, Separation, and Disposal of Plutonium and Other Actinides in High Level Radioactive Waste: The Effect of Temperature and Electrolyte Concentrations on Actinide Speciation	Lawrence Berkeley National Laboratory

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STCG Number: RL-WT053-S Containment Mobility Beneath Tank Farms **Site:** RL

Fundamental Science Need: (STCG Science Need)
Geoscience, geochemical, geophysical, chemical, and engineering science studies are needed to evaluation the importance of colloids in enhancing the migration of radionuclides, to characterize sorptive mechanisms of radionuclides to soil under extreme chemical conditions represented by tank effluents, and to combine known information into a computer model having temporal and spatial dependent variables with built-in degrees of uncertainty. This understanding and predictive ability is needed to characterize spread of contamination from leaking high level waste tanks.

Project Number:	Title	Institution:
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory

55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

Materials Science

STCG Number: RL-WT033-S Chemistry of Problem Constituents for HLW Virtrication **Site:** RL

Fundamental Science Need: (STCG Science Need) Fundamental chemical and material science studies are needed to characterize the solution thermodynamics of multicomponent borosilicate liquids with specific focus on effects of sodium, chromium, and phosphate as a function of concentration levels.

Project Number:	Title	Institution:
60296	Research Program to Investigate the Fundamental Chemistry of Technetium	Lawrence Berkeley National Laboratory
60362	Ion-Exchange Processes and Mechanisms in Glasses	Lawrence Berkeley National Laboratory

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STCG Number: RL-WT036-S Alternate Waste Form Development **Site:** RL

Fundamental Science Need: (STCG Science Need) Basic materials science investigations are needed to understand glass and ceramic structures and phase stabilization to develop alternative waste forms for high and low-level waste. Current baseline is borosilicate.

Project Number:	Title	Institution:
60118	Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms	Lawrence Livermore National Laboratory

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STCG Number: RL-WT041-S Radionuclide Partitioning **Site:** RL

Fundamental Science Need: (STCG Science Need) Chemical and engineering science studies are needed to understand, determine, or predict the partitioning of important radionuclides (especially Tc-99) among the waste processing solutions, suspended solids, and precipitates in these high ionic strength solutions so that efficient waste processes can be developed to reduce the volume of high level waste treated.

Project Number:	Title	Institution:
65398	Characterization of Actinides in Simulated Alkaline Tank Waste Sludges and Leach Solutions	Lawrence Berkeley National Laboratory

Project Number	Title	Institution
65352	Developing a Fundamental Basis for the Characterization, Separation, and Disposal of Plutonium and Other Actinides in High Level Radioactive Waste: The Effect of Temperature and Electrolyte Concentrations on Actinide Speciation	Lawrence Berkeley National Laboratory
60296	Research Program to Investigate the Fundamental Chemistry of Technetium	Lawrence Berkeley National Laboratory

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STCG Number: RL-WT046-S Getter Materials **Site:** RL

Fundamental Science Need: (STCG Science Need) Basic chemical, geochemical, and geoscience studies are desired to better understand binding of negatively charged elements and compounds with soil so that appropriate materials to retard transport of these chemicals can be determined.

Project Number:	Title	Institution:
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory

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STCG Number: RL-WT053-S Containment Mobility Beneath Tank Farms **Site:** RL

Fundamental Science Need: (STCG Science Need) Geoscience, geochemical, geophysical, chemical, and engineering science studies are needed to evaluation the importance of colloids in enhancing the migration of radionuclides, to characterize sorptive mechanisms of radionuclides to soil under extreme chemical conditions represented by tank effluents, and to combine known information into a computer model having temporal and spatial dependent variables with built-in degrees of uncertainty. This understanding and predictive ability is needed to characterize spread of contamination from leaking high level waste tanks.

Project Number:	Title	Institution:
55359	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone	Lawrence Berkeley National Laboratory
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory
54950	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes	Lawrence Livermore National Laboratory

Separations Chemistry

STCG Number: RL-WT041-S Radionuclide Partitioning **Site:** RL

Fundamental Science Need: (STCG Science Need) Chemical and engineering science studies are needed to understand, determine, or predict the partitioning of important radionuclides (especially Tc-99) among the waste processing solutions, suspended solids, and precipitates in these high ionic strength solutions so that efficient waste processes can be developed to reduce the volume of high level waste treated.

Project Number:	Title	Institution:
65352	Developing a Fundamental Basis for the Characterization, Separation, and Disposal of Plutonium and Other Actinides in High Level Radioactive Waste: The Effect of Temperature and Electrolyte Concentrations on Actinide Speciation	Lawrence Berkeley National Laboratory
65398	Characterization of Actinides in Simulated Alkaline Tank Waste Sludges and Leach Solutions	Lawrence Berkeley National Laboratory
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STCG Number: RL-WT046-S Getter Materials **Site:** RL

Fundamental Science Need: (STCG Science Need) Basic chemical, geochemical, and geoscience studies are desired to better understand binding of negatively charged elements and compounds with soil so that appropriate materials to retard transport of these chemicals can be determined.

Project Number:	Title	Institution:
55148	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry	Lawrence Livermore National Laboratory

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STCG Number: RL-WT048-S Inovative Methods for Radionuclide Separation **Site:** RL

Fundamental Science Need: (STCG Science Need) Fundamental chemical science investigations of the speciation of technetium and strontium are needed to develop process and techniques to remove these materials and reduce the volume of high and low level waste.

Project Number:	Title	Institution:
65352	Developing a Fundamental Basis for the Characterization, Separation, and Disposal of Plutonium and Other Actinides in High Level Radioactive Waste: The Effect of Temperature and Electrolyte Concentrations on Actinide Speciation	Lawrence Berkeley National Laboratory
65368	Speciation, Dissolution, and Redox Reactions of Chromium Relevant to Pretreatment and Separation of High-Level Tank Wastes	Lawrence Berkeley National Laboratory

65370	Actinide-Specific Interfacial Chemistry of Monolayer Coated Mesoporous Ceramics	Lawrence Berkeley National Laboratory